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MOFAT:
A TWO-DIMENSIONAL FINITE ELEMENT PROGRAM
FOR MULTIPHASE FLOW AND MULTICOMPONENT TRANSPORT

Program Documentation and User's Guide

by

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ABSTRACT

This report describes a two-dimensional finite element model for coupled multiphase flow and multicomponent transport in planar or radially symmetric vertical sections. Flow and transport of three fluid phases -- water, nonaqueous phase liquid (NAPL) and gas -- is considered by the program which also handles cases in which gas and/or NAPL phases are absent in part or all of the domain at any given time. The program will simulate flow only or coupled flow and transport. The flow module can be used to analyze two-phase flow of water and NAPL in a system with gas present but at constant pressure, or explicit three-phase flow of water, NAPL and gas at variable pressure. The transport module can handle up to five components which partition among water, NAPL, gas and solid phases assuming either local equilibrium interphase mass transfer or first-order kinetically controlled mass transfer. The governing equations are solved using an efficient upstream-weighted finite element scheme. Required input for flow analyses consists of initial conditions, soil hydraulic properties, fluid properties, time integration parameters, boundary condition data and mesh geometry. Three phase permeability-saturation-capillary pressure relations are defined by an extension of the van Genuchten model which considers effects of oil entrapment during periods of water imbibition. For transport analyses, additional input data are porous media dispersivities, initial water phase concentrations, equilibrium partition coefficients, component densities, diffusion coefficients, first-order decay coefficients, mass transfer coefficients (for nonequilibrium analyses) and boundary condition data. Time-dependent boundary conditions for the flow analysis may involve user-specified phase heads at nodes or phase fluxes along a boundary segment with zero-flux as the default condition. For transport analyses, initial conditions are specified in terms of equilibrium water phase concentrations of each partitionable component. Time-dependent boundary conditions may be stipulated as equilibrium water phase concentrations in the porous medium as prescribed fluxes defined in terms of a specified concentration in the influent liquid, or with zero dispersive flux specified. Program output consists of basic information on input parameters, mesh details and initial conditions plus pressure heads, saturations and velocities for each phase at every node for specified output intervals. For transport analyses, the phase concentrations at each node are output at each print-out interval.

CONTENTS

ABSTRACT	ii
CONTENTS	iii
FIGURES	v
1. INTRODUCTION	1
2. ANALYSIS OF MULTIPHASE FLOW	2
2.1 Mathematical model for multiphase flow	2
2.1.1 Governing equations	2
2.1.2 Initial and boundary conditions	3
2.1.3 Constitutive relations for flow model	4
2.2 Numerical model for flow equations	8
2.2.1 Finite element formulation	8
2.2.2 Treatment of nonlinearity	11
2.2.3 Convergence criteria and time-step control	13
2.2.4 Adaptive solution domain algorithm	14
2.3.5 Elimination of oil phase equation	14
3. ANALYSIS OF MULTICOMPONENT TRANSPORT	15
3.1 Mathematical model for transport	15
3.1.1 Governing phase transport equations	15
3.1.2 Phase-summed equation for local equilibrium transport	18
3.1.3 Consideration of nonequilibrium interphase mass transfer	20
3.1.4 Initial and boundary conditions	22
3.2 Numerical model description	24
3.2.1 General solution approach	24
3.2.2 Finite element formulation	26
3.2.3 Interphase mass transfer and density updating	29
4. GUIDE TO USE OF MOFAT	31
4.1 Estimation of soil and fluid properties	31
4.1.1 Soil properties	31
4.1.2 Bulk fluid properties	32
4.1.3 Component properties	35
4.2 Program structure and operation	38
4.2.1 Basic features and program control	38
4.2.2 Spatial discretization and mesh generation	42
4.2.3 Specification of initial conditions	43
4.2.4 Specification of boundary conditions	44
5. PROGRAM APPLICATIONS	48
5.1 Example 1. 1-D spill of two-component hydrocarbon	48
5.2 Example 2. 2-D planar spill with sloping water table	50

5.3 Example 3. 2-D radial dense solvent spill with vacuum extraction	51
6. REFERENCES	55
APPENDIX A. DESCRIPTION OF MAIN INPUT FILE	56
APPENDIX B. MAIN DATA FILE FOR EXAMPLE PROBLEM	68
APPENDIX C. MAIN OUTPUT FOR EXAMPLE PROBLEM	71
APPENDIX D. FLOW CHART FOR PROGRAM	98
APPENDIX E. DESCRIPTION OF PROGRAM SUBROUTINES	100
APPENDIX F. DESCRIPTION OF IMPORTANT PROGRAM VARIABLES	102

FIGURES

Figure 4.1.	Local side numbering of quadrilateral elements.	42
Figure 4.2.	Finite element mesh with numbers in parentheses indicating global element numbers and others referring to global node numbers.	43
Figure 5.1	Water and total liquid saturation vs depth at end of Stages 1, 2 and 3 for Example 1.	49
Figure 5.2	Aqueous xylene and toluene concentrations at outflow boundary for Example 1 for equilibrium and nonequilibrium analyses. Rate coefficients in d^{-1}	50
Figure 5.3	Oil saturation contours at the end of Stage 2 for Example 2.	51
Figure 5.4	Water phase concentration contours ($g\ m^{-3}$) at the end of Stage 2 for Example 2.	51
Figure 5.5	Gas phase concentration contours ($g\ m^{-3}$) at the end of Stage 2 for Example 2.	51
Figure 5.6	Oil saturation contours at the end of Stage 2 for Example 3.	53
Figure 5.7	Water saturation contours at the end of Stage 3 for Example 3.	53
Figure 5.8	PER mass in system vs time during Stage 3 of Example 3.	53

1. INTRODUCTION

This manual describes a two-dimensional finite element model, MOFAT, for coupled multiphase flow and multicomponent transport in planar or radially symmetric vertical sections. Flow and transport of three fluid phases—water, nonaqueous phase liquid (NAPL) and gas—is considered by the program which also handles cases in which gas and/or NAPL phases are absent in part or all of the domain at any given time.

The program allows the user to analyze flow only or coupled flow and transport. The flow module can be used to analyze two phase flow of water and NAPL in a system with gas present but at constant pressure, or explicit three phase flow of water, NAPL and gas at variable pressure. The transport module can handle up to five components which partition among water, NAPL, gas and solid phases assuming either local equilibrium interphase mass transfer or first-order kinetically controlled mass transfer. Time-lagged interphase mass transfer rates and phase densities are used to avoid costly iterative procedures between the flow and transport analyses while enabling accurate mass balance and providing for the effects of density-driven flow.

The systems of governing equations for multiphase flow and multicomponent transport are solved using an efficient upstream-weighted finite element scheme. To avoid costly numerical integration, an influence coefficient approach is utilized using linear rectangular elements. Nonlinear time integration in the flow analysis is handled using a Newton-Raphson method with an implicit saturation derivative formulation of the governing equations which is very efficient and accurate.

Required input for flow analyses consist of initial conditions, soil hydraulic properties, fluid properties, time integration parameters, boundary condition data and mesh geometry. Three phase permeability-saturation-capillary pressure relations are defined by an extension of the van Genuchten model which considers effects of oil entrapment during periods of water imbibition. The model requires specification of parameters defining the air-water capillary retention function, NAPL surface tension and interfacial tension with water, NAPL viscosity, NAPL density, maximum residual NAPL saturation and soil hydraulic conductivity. The latter may be anisotropic and soil properties may vary spatially.

For transport analyses, additional input data are porous media dispersivities, initial water phase concentrations, equilibrium partition coefficients, component densities, diffusion coefficients, first-order decay coefficients, mass transfer coefficients (for nonequilibrium analyses) and boundary condition data.

Initial conditions for the flow analysis are described by phase pressures expressed in terms of water-equivalent heights. If the analysis involves NAPL, the program has the capability to determine and assign NAPL heads which correspond to the zero oil saturation condition. Time-dependent boundary conditions for the flow analysis may involve user-specified phase heads at nodes (type-1 condition) or phase fluxes along a boundary segment (type-2 condition) with zero-

flux as the default condition. For transport analyses, initial conditions are specified in terms of equilibrium water phase concentrations of each partitionable component. Time-dependent boundary conditions may be stipulated as equilibrium water phase concentrations in the porous medium (type-1 condition) or as prescribed fluxes defined in terms of a specified concentration in the influent liquid (type-3 condition). The program assumes zero dispersive flux (type-2 condition) along any boundary segment not explicitly specified.

Program output consists of basic information on input parameters, mesh details and initial conditions plus pressure heads, saturations and velocities for each phase at every node for specified output intervals. In addition, the total volume or mass of each phase, time-step size and number of iterations are printed at each time-step. For transport analyses, the phase concentrations at each node are output at each print-out interval. The program allows the user to restart simulations from a previous run using an auxiliary data file automatically dumped from the previous simulation to define initial conditions for the restart problem.

Chapters 2 and 3 of this document describe the model development and numerical methods pertaining to multiphase flow and multicomponent transport, respectively. Chapter 4 discusses the estimation of soil and fluid properties required for the model and describes various practical aspects of program usage. Detailed instructions for creating the data file needed to run the program, and example input and output files are given in appendices.

2. ANALYSIS OF MULTIPHASE FLOW

2.1 Mathematical Model for Multiphase Flow

2.1.1 Governing equations

The mass conservation equations for water (w), organic liquid (o) and air (a), assuming an incompressible porous medium, incompressible liquid phases and compressible gas phase, may be written in summation convention for a two dimensional Cartesian domain as (*Parker, 1989*)

$$\phi \frac{\partial S_w}{\partial t} = - \frac{\partial q_{w_i}}{\partial x_i} + \frac{R_w}{\rho_w} \quad [2.1a]$$

$$\phi \frac{\partial S_o}{\partial t} = - \frac{\partial q_{o_i}}{\partial x_i} + \frac{R_o}{\rho_o} \quad [2.1b]$$

$$\phi \frac{\partial \rho_a S_a}{\partial t} = - \frac{\partial \rho_a q_{a_i}}{\partial x_i} + R_a \quad [2.1c]$$

where ϕ is porosity, S_p is the p- phase saturation, x_i (and x_j) are Cartesian spatial coordinates ($i, j = 1, 2$), q_{p_i} is the Darcy velocity of phase p in the i -direction, ρ_p is the density of phase p, R_p is the net mass transfer per unit porous media volume into (+) or out of (-) phase p, and t is the time.

Darcy velocities in the p-phase are defined by

$$q_{p_i} = - K_{p_{ij}} \left\{ \frac{\partial h_p}{\partial x_j} + \rho_{rp} u_j \right\} \quad [2.2]$$

where $K_{p_{ij}}$ is the p-phase conductivity tensor, $h_p = P_p / g \rho_w^*$ is the water height-equivalent pressure head of phase p where P_p is the p-phase pressure, g is gravitational acceleration and ρ_w^* is the density of pure water, ρ_p is the density of phase p, $\rho_{rp} = \rho_p / \rho_w^*$ is the p-phase specific gravity, and $u_j = \partial z / \partial x_j$ is a unit gravitational vector measured positive upwards where z is elevation.

Combining [2.1] and [2.2] yields

$$\phi \frac{\partial S_w}{\partial t} = \frac{\partial}{\partial x_i} \left[K_{w_{ij}} \left\{ \frac{\partial h_w}{\partial x_j} + \rho_{rw} u_j \right\} \right] + \frac{R_w}{\rho_w} \quad [2.3a]$$

$$\phi \frac{\partial S_o}{\partial t} = \frac{\partial}{\partial x_i} \left[K_{o_{ij}} \left\{ \frac{\partial h_o}{\partial x_j} + \rho_{ro} u_j \right\} \right] + \frac{R_o}{\rho_o} \quad [2.3b]$$

$$\phi \frac{\partial \rho_a S_a}{\partial t} = \frac{\partial}{\partial x_i} \left[\rho_a K_{a_{ij}} \left\{ \frac{\partial h_a}{\partial x_j} + \rho_{ra} u_j \right\} \right] + R_a \quad [2.3c]$$

If fluid saturations are treated as implicit functions of the phase pressures, equations [2.3] may be solved directly with phase pressures as primary variables. Details of the numerical methodology will be described in a subsequent section.

The system of flow equations solved may be reduced at the user's discretion. In many cases, gas pressure gradients may be regarded as negligible and the gas flow equation may be discarded. In this case, a gas phase may still be present and may be mobile, but it is assumed that gas flow has negligible effect on liquid flow due to small gas pressure gradients (Richard's assumption). The flow equations may be written also for the case of a two-dimensional radially symmetric domain using standard coordinate transformations. MOTRANS provides the capability to perform calculations for either Cartesian or radially symmetric domains. Options in the flow module can thus accommodate analyses for vertical plane slices (Cartesian symmetry) or vertical radial slices with two options for stipulation of the flow equations as follows:

- 1) Three phase flow of water, oil and gas phases (gas pressure variable)
- 2) Two phase liquid flow of water and oil (gas phase at atmospheric pressure)

Details of model development will be presented in this report for Case 1 with Cartesian geometry. Case 2 has an identical form to that of Case 1, but is degenerate in that the gas flow equation is omitted. The analysis of radial flow is likewise similar except for minor changes in the governing equations in converting them from Cartesian to radial symmetry.

2.1.2 Initial and boundary conditions

Initial conditions for each phase p must be stipulated on the entire flow domain R as

$$h_p(x_i, 0) = h_{p1}(x_i) \quad \text{on } R \text{ for } t = 0 \quad [2.4]$$

Boundary conditions may be stipulated as type-1 or type-2 as follows

$$h_p(x_i, t) = h_{p2}(x_i, t) \quad \text{on } S_1 \text{ for } t > 0 \quad [2.5a]$$

$$q_{p_i} n_i = \hat{q}_{p_i}(x_i, t) \quad \text{on } S_2 \text{ for } t > 0 \quad [2.5b]$$

Equation [2.5a] denotes type-1 boundary conditions (pressure head) on boundary region S_1 . The type-1 condition will commonly be used for the water phase on boundaries within a saturated aquifer where positive heads are specified corresponding to assumed vertical hydrostatic conditions (*i.e.*, $h_w = z_{wt} - z$ where z_{wt} is the water table elevation and h_w is the water head at elevation z). Type-1 conditions may also be used on infiltrating boundaries for water or oil if the infiltration is pressure controlled (*e.g.*, surface spill with free liquid on surface). Gas phase boundary conditions will often be type-1 corresponding to zero pressure along surfaces in contact with the atmosphere or at negative or positive heads at vacuum or injection points.

Equation [2.5b] denotes type-2 (fluid flux) boundary conditions with $\hat{q}_{p_i}(x_i, t)$ representing the normal flux on boundary segment S_2 for phase p with outward normal unit vector n_i . The default flow boundary condition is zero normal flux. Nonzero flux boundary conditions will be commonly used on boundary regions along which inflow rates are known. Specifying fluid removal rates is also possible, but may be somewhat troublesome since removal rates are often controlled by soil permeability to the phase which is not known *a priori*.

MOTRANS permits stipulation of type-1 or type-2 boundary conditions for all fluid phases independently using a very flexible scheme which utilizes user-defined schedules to specify time-dependent behavior. For problems run piecewise, a restart option is available. Mixed type boundary conditions can occur in certain problems, but are not considered directly. Such circumstances can arise, for example, when water or oil seeps from a boundary which is open to the atmosphere. The correct boundary conditions in such a case would involve stipulation of zero fluid flux as long as the boundary head remains negative, but switching to a type-1 condition with zero pressure after the pressure build up to atmospheric. To model such circumstances, the user will need to stop the code and restart it after manually changing the boundary conditions.

2.1.3 Constitutive relations for flow model

Relationships between phase permeabilities, saturations and pressures are described by a three phase extension of the van Genuchten model which takes into account effects of NAPL entrapment on NAPL relative permeability. To describe the saturation-capillary pressure relations, we introduce capillary pressure heads defined by

$$h_{aw} = h_a - h_w \quad [2.6a]$$

$$h_{ow} = h_o - h_w \quad [2.6b]$$

$$h_{ao} = h_a - h_o \quad [2.6c]$$

where $h_p = P_p / \rho_w g$ with P_p the p -phase pressure, ρ_w the density of water, and g the gravitational acceleration and $p = a$ (air), o (oil) or w (water).

Prior to the occurrence of oil at a given location, the system is treated as a two-phase air-water system described by the *van Genuchten* (1980) function

$$\bar{S}_w = [1 + (\alpha h_{aw})^n]^{-m} \quad [2.7]$$

where $\bar{S}_w = (S_w - S_m) / (1 - S_m)$ is the “effective” water saturation, S_m is the “irreducible” water saturation, α [L^{-1}] and n [-] are porous medium parameters and $m=1-1/n$.

Following the occurrence of oil at a location, the system is described by the three-phase relations

$$\bar{\bar{S}}_w = [1 + (\alpha \beta_{ow} h_{ow})^n]^{-m} \quad [2.8a]$$

$$\bar{S}_t = [1 + (\alpha \beta_{ao} h_{ao})^n]^{-m} \quad [2.8b]$$

where $\bar{\bar{S}}_w$ is the apparent water saturation, \bar{S}_t is the effective total liquid saturation, β_{ao} is a scaling coefficient which may be approximated by the ratio of water surface tension to oil surface tension and β_{ow} is a scaling factor approximated by the ratio of water surface tension to oil-water interfacial tension. The apparent water saturation is given by

$$\bar{\bar{S}}_w = \bar{S}_w + \bar{S}_{ot} \quad [2.9]$$

where \bar{S}_{ot} is the effective trapped oil saturation. The latter is estimated using an empirical relationship given by *Land* (1968) as

$$\bar{S}_{ot} = \left\{ \frac{1 - \bar{S}_w^{min}}{1 + R_{ow} (1 - \bar{S}_w^{min})} - \frac{1 - \bar{\bar{S}}_w}{1 + R_{ow} (1 - \bar{\bar{S}}_w)} \right\} \quad for \quad \bar{\bar{S}}_w > \bar{S}_w^{min} \quad [2.10a]$$

$$= 0 \quad for \quad \bar{\bar{S}}_w \leq \bar{S}_w^{min} \quad [2.10b]$$

where

$$R_{ow} = \frac{1}{\bar{S}_{ro}^{max}} - 1 \quad [2.10c]$$

where \bar{S}_{ro}^{max} is the maximum effective residual oil saturation where effective oil saturations are expressed in the form $S_o/(1-S_m)$. The minimum effective water saturation, \bar{S}_w^{min} , is defined as the historical minimum effective water saturation at a given location since changing from a two phase air-water to a three phase air-oil-water system. The value of \bar{S}_w^{min} is updated at the end of each time step after convergence and stored for each node. Actual water and oil saturations may be computed as

$$S_w = (1 - S_m) (\bar{S}_w - \bar{S}_{ot}) + S_m \quad [2.11a]$$

and

$$S_o = (1 - S_m) \bar{S}_t + S_m - S_w \quad [2.11b]$$

To avoid sudden discontinuities at a node due to the change from two phase air-water to three phase air-water-oil system under condition for which $1/\beta_{ao} + 1/\beta_{ow} \neq 1$, a node once classified as a three phase node will not be allowed to be considered as a two phase air-water node (*Kaluarachchi and Parker, 1989*). The necessary condition to classify a given node as a three phase node is

$$h_o > h_o^{cr} \quad [2.12a]$$

where

$$h_o^{cr} = \frac{\beta_{ao} h_a + \beta_{ow} h_w}{\beta_{ow} + \beta_{ao}} \quad [2.12b]$$

Phase conductivities are described by

$$K_{w_{ij}} = k_{rw} K_{S_{w_{ij}}} \quad [2.13a]$$

$$K_{o_{ij}} = k_{ro} K_{sw_{ij}} / \eta_{ro} \quad [2.13b]$$

$$K_{a_{ij}} = k_{ra} K_{sw_{ij}} / \eta_{ra} \quad [2.13c]$$

where k_{rp} is the relative permeability of phase p, η_{rp} is the absolute viscosity ratio between phase p and water, and $K_{sw_{ij}}$ is the saturated conductivity tensor for water. It is assumed that the coordinate system is oriented with the conductivity tensor, or otherwise that off-diagonal components may be disregarded, so that $K_{sw_{ij}} = 0$ for $i \neq j$.

Relative permeability relationships corresponding to the three phase van Genuchten model have been derived by *Parker et al.* (1987). These may be modified to account for effects of NAPL entrapment as described by *Kaluarachchi and Parker* (1991). The relative permeability relations are given by

$$k_{rw} = \bar{S}_w^{1/2} [1 - (1 - \bar{S}_w^{1/m})^m]^2 \quad [2.14a]$$

$$k_{ro} = (\bar{S}_t - \bar{S}_w)^{1/2} [(1 - \bar{S}_w^{1/m})^m - (1 - \bar{S}_t^{1/m})^m]^2 \quad [2.14b]$$

$$k_{ra} = (1 - \bar{S}_t)^{1/2} [1 - \bar{S}_t^{1/m}]^{2m} \quad [2.14c]$$

where parameters are all as previously defined for the saturation-pressure relations.

When gas phase flow is considered, the gas compressibility is described by the linear relation

$$\rho_a = \lambda h_a + \rho_a^o + \rho_a^c \quad [2.15]$$

where λ is the gas compressibility taken to be $1.17 \times 10^{-6} \text{ g cm}^{-4}$, ρ_a^o is the density of native soil air taken to be $1.12 \times 10^{-3} \text{ g cm}^{-3}$, and ρ_a^c is the density of contaminants in the gas phase which is determined from the solution to the transport model when coupled flow and transport is analyzed (see Chapter 3).

2.2 Numerical Model for Flow Equations

In this section, we describe the numerical model for the flow equations. The model description will be given for the case of fully three phase flow in a two-dimensional plane vertical slice. Analogous procedures are applied for the case of radial flow domains and for two phase flow with gas at atmospheric pressure.

2.2.1 Finite element formulation

The governing equations in this formulation have been solved using a finite element method with spatial derivative terms in the flow equations approximated by asymmetric upstream-weighting functions developed by *Huyakorn and Nilkuha* (1978), while the remaining terms are handled using linear basis functions. For efficiency, the model is restricted to the use of linear quadrilateral elements. The solutions for pressure heads over an element are approximated by trial functions of the form

$$h_w(x_i, t) = \sum_{I=1}^4 N_I(\xi, \eta) h_{wI}(t) \quad [2.16a]$$

$$h_o(x_i, t) = \sum_{I=1}^4 N_I(\xi, \eta) h_{oI}(t) \quad [2.16b]$$

$$h_a(x_i, t) = \sum_{I=1}^4 N_I(\xi, \eta) h_{aI}(t) \quad [2.16c]$$

where h_w , h_o and h_a are pressure heads for water, oil and air, respectively, at node I , N_I is the linear basis function for node I , and ξ and η are the local coordinates. Applying Green's theorem and the standard Galerkin principle to [2.3] with upstream-weighting for spatial terms yields

$$\begin{aligned} & \int_R K_{wi} \frac{\partial W_I}{\partial x_i} \frac{\partial N_I}{\partial x_i} h_{wJ} dR + \int_R K_{wi} \frac{\partial N_I}{\partial x_i} u_i dR \\ & + \int_R N_I N_J \frac{dS_{wJ}}{dt} dR + \int_s q_{nw} N_I dS = 0 \quad I, J = 1, 2, \dots, N \end{aligned} \quad [2.17a]$$

$$\begin{aligned} & \int_R K_{oi} \frac{\partial W_I}{\partial x_i} \frac{\partial N_I}{\partial x_i} h_{oJ} dR + \int_R K_{oi} \frac{\partial N_I}{\partial x_i} u_i dR \\ & + \int_R N_I N_J \frac{dS_{oJ}}{dt} dR + \int_s q_{no} N_I dS = 0 \quad I, J = 1, 2, \dots, N \end{aligned} \quad [2.17b]$$

$$\begin{aligned}
& \int_R \rho_a K_{a_i} \frac{\partial W_I}{\partial x_i} \frac{\partial N_I}{\partial x_i} h_{aJ} dR + \int_R \rho_a K_{a_i} \frac{\partial N_I}{\partial x_i} u_i dR \\
& + \int_R N_I N_J \frac{d(\rho_a S_{aJ})}{dt} dR + \int_s q_{na} N_I dS = 0 \quad I, J = 1, 2, \dots, N
\end{aligned} \tag{2.17c}$$

where W_I is an upstream-weighted shape function described in detail by *Kaluarachchi and Parker* (1989) and N is the number of nodes in the domain. Since only diagonal terms in the conductivity tensor are considered in the present analysis, the double subscript notation is henceforth dropped.

Following *Kaluarachchi and Parker* (1989), we expand the matrices in the first two integrals of [2.17a], [2.17b] and [2.17c] into four submatrices by permitting the hydraulic conductivity within an element to vary through the upstream-weighting function such that

$$K_{p_i}(x_i, t) = \sum_{I=1}^4 W_I(\xi, \eta) K_{p_i}^I \tag{2.18}$$

where $K_{p_i}^I$ denotes the hydraulic conductivity attributed to node I . In the present analysis, we take $K_{p_i}^I$ values corresponding exactly to node points. Substituting [2.18] into [2.17] and integrating gives

$$A_{wIJ} h_{wJ} + B_{IJ} \frac{dS_{wJ}}{dt} - F_{wI} = 0 \tag{2.19a}$$

$$A_{oIJ} h_{oJ} + B_{IJ} \frac{dS_{oJ}}{dt} - F_{oI} = 0 \tag{2.19b}$$

$$A_{aIJ} h_{aJ} + B_{IJ} \frac{d(\rho_a S_{aJ})}{dt} - F_{aI} = 0 \tag{2.19c}$$

where

$$A_{wIJ} = \sum_{e=1}^n \left(\frac{m}{d} \sum_{I=1}^4 [U^x]_I^e K_{w_x}^I + \frac{d}{m} \sum_{g=1}^4 [U^y]_I^e K_{w_y}^I \right) \quad [2.20a]$$

$$A_{oIJ} = \sum_{e=1}^n \left(\frac{m}{d} \sum_{I=1}^4 [U^x]_I^e K_{o_x}^I + \frac{d}{m} \sum_{g=1}^4 [U^y]_I^e K_{o_y}^I \right) \quad [2.20b]$$

$$A_{aIJ} = \sum_{e=1}^n \left(\frac{m}{d} \sum_{I=1}^4 [U^x]_I^e K_{a_x}^I + \frac{d}{m} \sum_{g=1}^4 [U^y]_I^e K_{a_y}^I \right) \quad [2.20c]$$

$$B_{IJ} = \phi \sum_{e=1}^n \frac{md}{4} \quad [2.20d]$$

$$F_{wI} = - \sum_{e=1}^n \frac{d}{2} \sum_{I=1}^4 [G]_I^e K_{w_y}^I + \text{boundary flux term} \quad [2.20e]$$

$$F_{oI} = - \sum_{e=1}^n \frac{d}{2} \rho_{ro} \sum_{I=1}^4 [G]_I^e K_{o_y}^I + \text{boundary flux term} \quad [2.20f]$$

$$F_{aI} = - \sum_{e=1}^n \frac{d}{2} \rho_{ra} \sum_{I=1}^4 [G]_I^e K_{a_y}^I + \text{boundary flux term} \quad [2.20g]$$

where m and d are the width and length of the rectangular element respectively. Influence coefficient matrices, $[U^x]_I^e$, $[U^y]_I^e$, $[G]_I^e$ and coefficient vectors for boundary flux terms are given by *Kaluarachchi and Parker (1989)*. In the subsequent analysis the boundary flux terms in [2.20e] - [2.20g] have been omitted for simplicity. A mass lumping procedure is employed to diagonalize the mass storage matrix.

2.2.2 Treatment of nonlinearity

A Newton-Raphson iteration method is used with this formulation to solve the nonlinear problem. In residual form, [2.19] may be written as

$$r_{w_I} = A_{w_I J} h_{w_J} + B_{I J} \frac{d S_{w_J}}{d t} - F_{w_I} \quad [2.21a]$$

$$r_{o_I} = A_{o_I J} h_{o_J} + B_{I J} \frac{d S_{o_J}}{d t} - F_{o_I} \quad [2.21b]$$

$$r_{a_I} = A_{a_I J} h_{a_J} + B_{I J} \frac{d (\rho_{a_J} S_{a_J})}{d t} - F_{a_I} \quad [2.21c]$$

Applying the Newton-Raphson procedure to [2.21] gives

$$\begin{aligned} \frac{\partial r_{w_I}}{\partial h_{w_J}} (h_{w_J}^{r+1} - h_{w_J}^r) + \frac{\partial r_{w_I}}{\partial h_{o_J}} (h_{o_J}^{r+1} - h_{o_J}^r) \\ + \frac{\partial r_{w_I}}{\partial h_{a_J}} (h_{a_J}^{r+1} - h_{a_J}^r) = - r_{w_I}^r \end{aligned} \quad [2.22a]$$

$$\begin{aligned} \frac{\partial r_{o_I}}{\partial h_{w_J}} (h_{w_J}^{r+1} - h_{w_J}^r) + \frac{\partial r_{o_I}}{\partial h_{o_J}} (h_{o_J}^{r+1} - h_{o_J}^r) \\ + \frac{\partial r_{o_I}}{\partial h_{a_J}} (h_{a_J}^{r+1} - h_{a_J}^r) = - r_{o_I}^r \end{aligned} \quad [2.22b]$$

$$\begin{aligned} \frac{\partial r_{a_I}}{\partial h_{w_J}} (h_{w_J}^{r+1} - h_{w_J}^r) + \frac{\partial r_{a_I}}{\partial h_{o_J}} (h_{o_J}^{r+1} - h_{o_J}^r) \\ + \frac{\partial r_{a_I}}{\partial h_{a_J}} (h_{a_J}^{r+1} - h_{a_J}^r) = - r_{a_I}^r \end{aligned} \quad [2.22c]$$

where r and $r+1$ refer to the previous and current iterations, respectively. The derivatives in [2.22] can be expressed as

$$\frac{\partial r_{wI}}{\partial h_{wJ}} = A_{wIJ} + h_{wL} \frac{\partial A_{wIL}}{\partial h_{wJ}} + [B_{IJ} \frac{\partial S_{wJ}}{\partial h_{wJ}}] / \Delta t - \frac{\partial F_{wI}}{\partial h_{wJ}} \quad [2.23a]$$

$$\frac{\partial r_{wI}}{\partial h_{oJ}} = h_{wL} \frac{\partial A_{wIL}}{\partial h_{oJ}} + [B_{IJ} \frac{\partial S_{wJ}}{\partial h_{oJ}}] / \Delta t - \frac{\partial F_{wI}}{\partial h_{oJ}} \quad [2.23b]$$

$$\frac{\partial r_{wI}}{\partial h_{aJ}} = h_{wL} \frac{\partial A_{wIL}}{\partial h_{aJ}} + [B_{IJ} \frac{\partial S_{wJ}}{\partial h_{aJ}}] / \Delta t - \frac{\partial F_{wI}}{\partial h_{aJ}} \quad [2.23c]$$

$$\frac{\partial r_{oI}}{\partial h_{wJ}} = h_{oL} \frac{\partial A_{oIL}}{\partial h_{wJ}} + [B_{IJ} \frac{\partial S_{oJ}}{\partial h_{wJ}}] / \Delta t - \frac{\partial F_{oI}}{\partial h_{wJ}} \quad [2.23d]$$

$$\frac{\partial r_{oI}}{\partial h_{oJ}} = A_{oIJ} + h_{oL} \frac{\partial A_{oIL}}{\partial h_{oJ}} + [B_{IJ} \frac{\partial S_{oJ}}{\partial h_{oJ}}] / \Delta t - \frac{\partial F_{oI}}{\partial h_{oJ}} \quad [2.23e]$$

$$\frac{\partial r_{oI}}{\partial h_{aJ}} = h_{oL} \frac{\partial A_{oIL}}{\partial h_{aJ}} + [B_{IJ} \frac{\partial S_{oJ}}{\partial h_{aJ}}] / \Delta t - \frac{\partial F_{oI}}{\partial h_{aJ}} \quad [2.23f]$$

$$\frac{\partial r_{aI}}{\partial h_{wJ}} = h_{aL} \frac{\partial A_{aIL}}{\partial h_{wJ}} + [B_{IJ} \frac{\partial (\rho_{aJ} S_{aJ})}{\partial h_{wJ}}] / \Delta t - \frac{\partial F_{aI}}{\partial h_{wJ}} \quad [2.23g]$$

$$\frac{\partial r_{aI}}{\partial h_{oJ}} = h_{aL} \frac{\partial A_{aIL}}{\partial h_{oJ}} + [B_{IJ} \frac{\partial S_{aJ}}{\partial h_{oJ}}] / \Delta t - \frac{\partial F_{aI}}{\partial h_{oJ}} \quad [2.23h]$$

$$\frac{\partial r_{aI}}{\partial h_{aJ}} = A_{aIJ} + h_{aL} \frac{\partial A_{aIL}}{\partial h_{aJ}} + [B_{IJ} \frac{\partial S_{aJ}}{\partial h_{aJ}}] / \Delta t - \frac{\partial F_{aI}}{\partial h_{aJ}} \quad [2.23i]$$

where $\Delta t = t^{p+1} - t^p$ and the subscript L is a dummy index denoting the appropriate influence coefficient matrix to be selected for a particular set of I and J . In [2.21], ds_{wJ} , ds_{oJ} and ds_{aJ} are changes in the water, oil and air saturations, respectively, over the time interval calculated as

$$ds_{wJ} = S_{wJ}^{t+1} - S_{wJ}^t \quad [2.24a]$$

$$ds_{oJ} = S_{oJ}^{t+1} - S_{oJ}^t \quad [2.24b]$$

$$ds_{aJ} = S_{aJ}^{t+1} - S_{aJ}^t \quad [2.24c]$$

where t and $t+1$ denote previous and current time-steps. Phase saturations are calculated from phase pressures using the constitutive relations described earlier. Saturations at the $t+1$ time-step in [2.24] as well as residuals r_{wI} and r_{oI} in [2.21] and derivatives with respect to pressure heads in [2.23] are evaluated using currently updated pressures for the present time-step. Equation [2.22] is then solved for the changes in pressure heads, the nodal pressure heads are updated, and the procedure is iterated until the solution converges.

2.2.3 Convergence criteria and time-step control

The convergence criterion for phase p ($= o, w, a$) is as follows

$$|h_p^{r+1} - h_p^r| \leq |h_p^r| \epsilon_r + \epsilon_a \quad [2.25]$$

where $r+1$ and r refer to current and previous iterations, ϵ_r is the allowable relative convergence error and ϵ_a is the allowable absolute convergence error for phase p . The convergence criteria must be met for all phases and at all nodes.

Automatic adjustment of the time-step size is undertaken depending on the number of iterations required for nonlinear convergence relative to a specified maximum number of iterations, I_{max} , given by the user. If the number of iterations is less than or equal to $I_{max}/4$ the time-step size is increased by a factor F for the next time-step. If the number of iterations exceeds $I_{max}/3$ but is less than I_{max} , the solution proceeds to the next time step but the time step size is decreased by a factor F . If the number of iterations exceeds I_{max} , program execution is halted and output is dumped to enable the problem to be restarted (*e.g.*, after reducing the time-step size). For most simulations, good results may be obtained using $I_{max} = 30$ and $F = 1.03$ to 1.05 .

2.2.4 Adaptive solution domain algorithm

In many practical problems involving soil contamination with immiscible organic liquids, a substantial part of the spatial domain may exhibit negligible changes in fluid saturations over all or part of the time domain. For example, during infiltration of oil, the region well ahead of an oil front may be essentially static. Also, after redistribution proceeds to the point "residual saturations" are achieved or under steady flow boundary conditions, quasi-static or steady-state conditions may occur which lead to subregions with negligible changes in fluid pressures and saturations. Solution of the flow equations in such subregions involves unnecessary computational effort. An adaptive solution domain (ASD) formulation was developed to confine the mathematical solution domain to a subdomain within which transient oil flow occurs in order to improve computational efficiency. The method involves reducing the solution domain for the water and oil flow equations by eliminating from the global matrix assembly elements which are not experiencing significant changes in fluid saturations and/or pressures. The formulation achieves computational efficiency by solving the flow equations only for the part of the domain where changes in fluid pressure or the saturations take place above stipulated tolerances.

In the ASD method, elements are categorized as either "active" or "inactive" at a given iteration. If the element is classified as active, then it is included in the global matrix assembly, otherwise it is excluded. The criteria for changing a node from inactive to active is based on the changes in water pressure head, oil pressure head, oil saturation, and water saturation at connected nodes from the last converged time-step to the current iteration. The specific criteria for changing an element from inactive to active is as follows

$$\Delta h_w > TOL1 \quad [2.26a]$$

or

$$\Delta h_o > TOL1 \quad [2.26b]$$

or

$$\Delta S_w > TOL2 \quad [2.26c]$$

or

$$\Delta S_o > TOL2 \quad [2.26d]$$

where Δh_w , Δh_o , ΔS_w and ΔS_o are the changes in h_w , h_o , S_w and S_o , respectively, between the previous converged time-step and the current iteration, TOL1 is a specified head tolerance for the ASD method and TOL2 is a specified saturation tolerance. Equations for nodes on the active-inactive frontier will have contributions only from active elements and the boundary will shift naturally as imbibition or drainage "fronts" pass through the domain.

2.3.5 Elimination of oil phase equation

In many practical situations involving flow of organic liquids, the oil phase fluxes after long redistribution periods become negligible, resulting in insignificant changes in oil phase saturations

within the entire domain. MOTRANS has an option to globally eliminate the oil equation from the solution if changes in oil saturation at all nodes during the current time step are smaller than tolerance TOL3.

3. ANALYSIS OF MULTICOMPONENT TRANSPORT

3.1 Mathematical Model for Transport

3.1.1 Governing phase transport equations

In this chapter, we will describe a model for transport of NAPL constituents which can partition among water, oil, air and solid phases following *Parker (1989)* and *Kaluarachchi and Parker (1990)*. To model component transport, continuity and mass flux equations for each partitionable component in each phase must be specified. Mass conservation of species α in the p-phase requires that

$$\phi \frac{\partial C_{\alpha p} S_p}{\partial t} = - \frac{\partial J_{\alpha p i}}{\partial x_i} + R_{\alpha p} + Y_{\alpha p} \quad [3.1]$$

where $C_{\alpha p}$ is the concentration of the noninert α component in p-phase expressed as the mass of α per phase volume [$M L^{-3}$], $J_{\alpha p i}$ is the mass flux density of α in p-phase per porous media cross section in the i-direction [$M L^{-2} T^{-1}$], $R_{\alpha p}$ is the net mass transfer rate per porous medium volume of species α into (+) or out of (-) the p-phase [$M L^{-3}$], and $Y_{\alpha p}$ is the net production (+) or decay (-) of α within phase p per porous medium volume due to reactions within the p-phase [$M L^{-3}$] described subsequently by

$$Y_{\alpha p} = - \mu_{\alpha p} C_{\alpha p} \quad [3.2]$$

where $\mu_{\alpha p}$ is an apparent first-order decay coefficient.

The mass flux density of component α in phase p due to convection, diffusion and mechanical dispersion is described by

$$J_{\alpha p i} = C_{\alpha p} q_{p i} - \phi S_p D_{\alpha p i j} \frac{\partial C_{\alpha p}}{\partial x_j} \quad [3.3]$$

where $D_{\alpha p i j}$ is a dispersion tensor given by

$$D_{\alpha p i j} = \sigma_{\alpha p} (D_{\alpha p}^{dif} + D_{p i j}^{hyd}) \quad [3.4]$$

in which $D_{\alpha p}^{dif}$ is the molecular diffusion coefficient of α in the p-phase of the porous medium, $D_{p i j}^{hyd}$

is a mechanical dispersion coefficient, and g_{ap} is a nondilute solution correction factor. For the case of transport of low solubility organic components, small volume fractions of organic components in water and gaseous phases will occur and $g_{\alpha w} = g_{\alpha a} = 1$ is assumed. For nonaqueous phase liquids, the phase composition may reach 100% (e.g., single component organic liquid) at which point dispersive transport becomes nonexistent. We accommodate nondilute solution diffusion-dispersion by approximating the oil phase nonideal solution factor by

$$g_{\alpha o} = 1 - \frac{C_{\alpha o}}{\rho_o} \quad [3.5]$$

Employing the tortuosity model of *Millington and Quirk* (1959) yields the expression for $D_{\alpha p}^{dif}$ as

$$D_{\alpha p}^{dif} = \phi^{1/3} S_p^{7/3} D_{\alpha p}^o \quad [3.6]$$

where $D_{\alpha p}^o$ is the diffusion coefficient of α in bulk p-phase. The mechanical dispersion coefficient is shown by *Bear* (1972) to have the form

$$D_{p i j}^{hyd} = \frac{1}{\phi S_p} [A_T \bar{q}_p \delta_{ij} + (A_L - A_T) \frac{|q_{pi} q_{pj}|}{\bar{q}_p}] \quad [3.7]$$

where A_L and A_T are longitudinal and transverse dispersivities [L], q_{pi} and q_{pj} are p-phase Darcy velocities in the i and j directions, $\bar{q}_p = |\sum q_{pi}^2|^{1/2}$ is the absolute magnitude of the p-phase velocity, and δ_{ij} is Kroonecker's delta.

Combining the phase continuity equation [3.1] and the mass flux equation [3.3] for transport of component α in the p-phase yields

$$\phi \frac{\partial C_{\alpha p} S_p}{\partial t} = \frac{\partial}{\partial x_i} [\phi S_p D_{\alpha p i j} \frac{\partial C_{\alpha p}}{\partial x_j}] - \frac{\partial C_{\alpha p} q_{pi}}{\partial x_i} + R_{\alpha p} - \mu_{\alpha p} C_{\alpha p} \quad [3.8]$$

Expanding the first and third terms in [3.8], employing the bulk p-phase continuity equation [2.1], and assuming density derivative terms to be of second order importance within a given time step yields

$$\phi S_p \frac{\partial C_{\alpha p}}{\partial t} = \frac{\partial}{\partial x_i} \left[\phi S_p D_{\alpha p i j} \frac{\partial C_{\alpha p}}{\partial x_j} \right] - q_{p i} \frac{\partial C_{\alpha p}}{\partial x_i} + R_{\alpha p} - \left(\mu_{\alpha p} + \frac{R_p}{\rho_p} \right) C_{\alpha p} \quad [3.9]$$

where the total phase mass transfer rate, R_p , it may be noted, is related to the individual component mass transfer rates by

$$R_p = \sum_{\alpha=1}^{n_s} R_{\alpha p} \quad [3.10]$$

where n, denotes the number of "noninert" or partitionable species. In the present context, we will use the term "inert" to refer to components of the NAPL phase which are for practical purposes insoluble and nonvolatile. For the three fluid phase system, [3.9] constitutes a system of three equations which we may write for the water phase (p=w), the organic liquid phase (p=o) and the gas phase (p=a) as

$$\phi S_w \frac{\partial C_{\alpha w}}{\partial t} = \frac{\partial}{\partial x_i} \left[\phi S_w D_{\alpha w i j} \frac{\partial C_{\alpha w}}{\partial x_j} \right] - q_{w i} \frac{\partial C_{\alpha w}}{\partial x_i} + R_{\alpha w} - \left(\mu_{\alpha w} + \frac{R_w}{\rho_w} \right) C_{\alpha w} \quad [3.11a]$$

$$\phi S_o \frac{\partial C_{\alpha o}}{\partial t} = \frac{\partial}{\partial x_i} \left[\phi S_o D_{\alpha o i j} \frac{\partial C_{\alpha o}}{\partial x_j} \right] - q_{o i} \frac{\partial C_{\alpha o}}{\partial x_i} + R_{\alpha o} - \left(\mu_{\alpha o} + \frac{R_o}{\rho_o} \right) C_{\alpha o} \quad [3.11b]$$

$$\phi S_a \frac{\partial C_{\alpha a}}{\partial t} = \frac{\partial}{\partial x_i} \left[\phi S_a D_{\alpha a i j} \frac{\partial C_{\alpha a}}{\partial x_j} \right] - q_{a i} \frac{\partial C_{\alpha a}}{\partial x_i} + R_{\alpha a} - \left(\mu_{\alpha a} + \frac{R_a}{\rho_a} \right) C_{\alpha a} \quad [3.11c]$$

To accommodate adsorption of α by the solid phase, an additional continuity equation is required which may be written as

$$\frac{\partial C_{\alpha s}}{\partial t} = R_{\alpha s} - \mu_{\alpha s} C_{\alpha s} \quad [3.12]$$

where $C_{\alpha s}$ is the solid phase concentration expressed as mass of adsorbed component α per porous medium volume [$M L^{-3}$], $\mu_{\alpha s}$, is the first-order decay coefficient (T^{-1}) in the solid phase and $R_{\alpha s}$, is the mass transfer rate per porous medium volume to (+) or from (-) the solid phase [$M L^{-3} T^{-1}$].

3.1.2 Phase-summed equations for local equilibrium transport

Coupling between the phase transport equations arises due to the interphase transfer terms. Explicit consideration of interphase transfer kinetics may often be justifiably avoided by assuming phase transfer to be equilibrium controlled. We consider first the case of linear partitioning and introduce the approximate thermodynamic relations

$$C_{\alpha o} = \Gamma_{\alpha o} C_{\alpha w} \quad [3.13a]$$

$$C_{\alpha a} = \Gamma_{\alpha a} C_{\alpha w} \quad [3.13b]$$

$$C_{\alpha s} = \Gamma_{\alpha s} C_{\alpha w} \quad [3.13c]$$

where $\Gamma_{\alpha o}$ is the equilibrium partition coefficient for species α between water and organic liquid (Raoult's constant), $\Gamma_{\alpha a}$ is the equilibrium partition coefficient between water and gas (Henry's constant), and $\Gamma_{\alpha s}$ is a dimensionless equilibrium partition coefficient between water and solid phase. Using the equilibrium relations, we may rewrite the phase transport equations in terms of a single phase concentration. For water-wet systems, it is logical to retain the water phase concentration, since water will always be present in the system. Using [3.13] to eliminate oil, gas and solid phase concentrations from [3.11] and summing the equations noting that

$$R_{\alpha w} + R_{\alpha o} + R_{\alpha s} + R_{\alpha a} = 0 \quad [3.14]$$

leads to the α -component phase-summed transport equation in terms of water phase concentrations

$$\phi_{\alpha}^* \frac{\partial C_{\alpha w}}{\partial t} = \frac{\partial}{\partial x_i} \left[D_{\alpha i j}^* \frac{\partial C_{\alpha w}}{\partial x_j} \right] - q_{\alpha i}^* \frac{\partial C_{\alpha w}}{\partial x_i} - \mu_{\alpha}^* C_{\alpha w} \quad [3.15a]$$

where

$$\phi_{\alpha}^* = \phi S_w + \phi S_o \Gamma_{\alpha o} + \phi S_a \Gamma_{\alpha a} + \Gamma_{\alpha s} \quad [3.15b]$$

$$D_{\alpha i j}^* = \phi S_w D_{\alpha w i j} + \phi S_o D_{\alpha w i j} \Gamma_{\alpha o} + \phi S_a D_{\alpha w i j} \Gamma_{\alpha a} \quad [3.15c]$$

$$q_{\alpha i}^* = q_{w i} + q_{o i} \Gamma_{\alpha o} + q_{a i} \Gamma_{\alpha a} \quad [3.15d]$$

$$\mu_{\alpha}^* = \mu_{\alpha w} + \mu_{\alpha o} \Gamma_{\alpha o} + \mu_{\alpha a} \Gamma_{\alpha a} + \mu_{\alpha s} \Gamma_{\alpha s} + \frac{R_w}{\rho_w} + \frac{R_o \Gamma_{\alpha o}}{\rho_o} + \frac{R_a \Gamma_{\alpha a}}{\rho_a} \quad [3.15e]$$

Note that [3.15] has the same form as the simple single phase transport equation. However, the coefficients represent pooled effects of transport in all phases. Note also that interphase mass transfer terms occur in the phase summed equation only as a sum over all components. An alternative form of the phase-summed transport equation may be written in terms of the oil phase species concentrations. The α -component phase-summed transport equation in terms of oil phase concentrations has the form

$$\phi_{\alpha}^{**} \frac{\partial C_{\alpha o}}{\partial t} = \frac{\partial}{\partial x_i} \left[D_{\alpha ij}^{**} \frac{\partial C_{\alpha o}}{\partial x_j} \right] - q_{\alpha i}^{**} \frac{\partial C_{\alpha o}}{\partial x_i} - \mu_{\alpha}^{**} C_{\alpha o} \quad [3.16a]$$

where

$$\phi_{\alpha}^{**} = \phi S_o + \frac{\phi S_w}{\Gamma_{\alpha o}} + \frac{\phi S_a \Gamma_{\alpha a}}{\Gamma_{\alpha o}} + \frac{\Gamma_{\alpha s}}{\Gamma_{\alpha o}} \quad [3.16b]$$

$$D_{\alpha ij}^{**} = \phi S_o D_{\alpha o ij} + \frac{\phi S_w D_{\alpha w ij}}{\Gamma_{\alpha o}} + \frac{\phi S_a D_{\alpha a ij} \Gamma_{\alpha a}}{\Gamma_{\alpha a}} \quad [3.16c]$$

$$q_{\alpha i}^{**} = q_{oi} + \frac{q_{wi}}{\Gamma_{\alpha o}} + \frac{q_{ai} \Gamma_{\alpha a}}{\Gamma_{\alpha a}} \quad [3.16d]$$

$$\mu_{\alpha}^{**} = \mu_{\alpha o} + \frac{\mu_{\alpha w}}{\Gamma_{\alpha o}} + \frac{\mu_{\alpha a} \Gamma_{\alpha a}}{\Gamma_{\alpha a}} + \frac{\mu_{\alpha s} \Gamma_{\alpha s}}{\Gamma_{\alpha a}} + \frac{R_o}{\rho_o} + \frac{R_w}{\rho_w \Gamma_{\alpha o}} + \frac{R_a \Gamma_{\alpha a}}{\rho_a \Gamma_{\alpha o}} \quad [3.16e]$$

The form of the oil-based equation is identical to that of the water-based phase-summed equation. The water-based equation has the conceptual advantage that $C_{\alpha w}$ is physically meaningful at all locations in the porous medium, whereas $C_{\alpha o}$ only has physical meaning at locations where $S_o > 0$. The latter constraint, however, imposes no mathematical difficulty since [3.13] can in any event be employed as a *definition* of $C_{\alpha o}$ as well as $C_{\alpha a}$ whether or not the phase exists. MOTRANS includes provisions for solution of either the water- or oil-based phase-summed transport equations. Since most of the species mass commonly resides in the oil phase, the oil-based equation has the advantage that mass balance accuracy of the solution may be more readily controlled.

When simulating two phase liquid flow consisting of water and oil with constant gas pressure, only diffusive transport is considered in the gas phase— i.e., $q_a = 0$ is assumed for this case. It should be noted that even if gas pressure gradients have negligible effect on liquid phase flow, this does not strictly imply zero gas flow. If fluid saturations change in time, gas flow will occur. Furthermore, phase partitioning may result in density gradients in the gas phase which can induce significant flow.

3.1.3 Consideration of nonequilibrium interphase mass transfer

The phase-summed formulation of the transport equations may be generalized to account for nonequilibrium phase partitioning by introducing the concept of *apparent partition coefficients*. Under transient field conditions, at a given location in time and space, actual phase concentration ratios may differ from the true equilibrium ratios defined by [3.13]. With this in mind, we define apparent partition coefficients—which will vary in time and space—by analogs of [3.13] as

$$C_{\alpha o} = \Gamma'_{\alpha o} C_{\alpha w} \quad [3.17a]$$

$$C_{\alpha a} = \Gamma'_{\alpha a} C_{\alpha w} \quad [3.17b]$$

$$C_{\alpha s} = \Gamma'_{\alpha s} C_{\alpha w} \quad [3.17c]$$

For any two phases which are in physical contact, the rate of mass transfer will be described by first order mass transfer functions of the form

$$R_{\alpha 12} = k_{\alpha 12} (C_{\alpha 1} - C_{\alpha 1}^e) \quad [3.18a]$$

$$= - k_{\alpha 12} (C_{\alpha 2} - C_{\alpha 2}^e) \quad [3.18b]$$

where $R_{\alpha 12}$ is the rate of mass transfer of α per porous medium volume from phase 1 to phase 2, $C_{\alpha 1}$ is the actual concentration of α in phase 1, $C_{\alpha 1}^e$ is the concentration of which would occur in phase 1 if it were in equilibrium with phase 2, $C_{\alpha 2}$ is the actual concentration of α in phase 2, $C_{\alpha 2}^e$ is the concentration of α that would occur in phase 2 if it were in equilibrium with phase 1, and $k_{\alpha 12}$ is a mass transfer rate coefficient [T^{-1}].

Consider first, the case of mass transfer between oil and water phases when both phases exist at a point in time and space. Employing [3.18a] along with [3.17a] for the actual oil phase concentration and [3.13a] for the equilibrium concentration gives

$$R_{\alpha o w} = k_{\alpha o w} (\Gamma'_{\alpha o} C_{\alpha w} - \Gamma_{\alpha o} C_{\alpha w}) \quad [3.19]$$

which may be solved in terms of $\Gamma'_{\alpha o}$ as

$$\Gamma'_{\alpha o} = \Gamma_{\alpha o} + \frac{R_{\alpha o w}}{k_{\alpha o w} C_{\alpha w}} \quad [3.20]$$

which indicates that the apparent partition coefficient may be expressed as the actual partition coefficient plus a correction term which depends on the sign and magnitude of the actual mass transfer rate and on the concentration in the water phase.

If free oil is present in the system at a given point in time and space, so that air and oil are physically in contact, mass transfer between oil and gas phases may be described in a similar fashion. Employing in this case [3.18b] we obtain

$$R_{\alpha o a} = -k_{\alpha o a} (\Gamma'_{\alpha a} C_{\alpha w} - \Gamma_{\alpha a} C_{\alpha w}) \quad [3.21]$$

which yields

$$\Gamma'_{\alpha a} = \Gamma_{\alpha a} - \frac{R_{\alpha o a}}{k_{\alpha o a} C_{\alpha w}} \quad [3.22]$$

In the absence of free oil in the porous medium at a given location, mass transfer will occur between water and gas phases rather than between oil and gas phases. Proceeding in the same manner as for oil-gas mass transfer yields

$$\Gamma'_{\alpha a} = \Gamma_{\alpha a} - \frac{R_{\alpha w a}}{k_{\alpha w a} C_{\alpha w}} \quad [3.23]$$

Note that either [3.22] or [3.23] will be relevant at a given location and time, depending on whether free oil occurs. Finally, mass transfer between water and solid phase may be considered by employing [3.18b] to obtain

$$\Gamma'_{\alpha s} = \Gamma_{\alpha s} - \frac{R_{\alpha ws}}{k_{\alpha ws} C_{\alpha w}} \quad [3.24]$$

In order to describe transport with nonequilibrium phase partitioning, the individual phase transport equations, [3.11a-c] and [3.12], may be summed as described in section 3.1.2 but using apparent rather than equilibrium partition coefficients. Thus [3.15] will hold for the nonequilibrium case with apparent partition coefficients used in lieu of the equilibrium coefficients. Nonlinearity is introduced into the resulting phase-summed transport equation due to the dependence of apparent partition coefficients on concentration as well as mass transfer rates. Thus, an iterative solution procedure will be required for the nonequilibrium problem as will be discussed later.

If the transport equations are written in terms of oil phase concentrations; similar expressions to those given above may be derived to define apparent partition coefficients as functions of mass transfer rates and oil phase concentrations.

3.1.4 Initial and boundary conditions

Since the transport equation is written in the phase-summed form, it is necessary to specify initial and boundary conditions in terms of a single concentration. In the following, as well as in the program itself, we will specify initial conditions and type-1 boundary conditions in terms of water phase concentrations. If the oil concentration form of the phase-summed transport equation is employed, oil phase concentrations are internally computed from the specified water phase values and the equilibrium relations. Type-3 or flux-type boundary conditions are defined in terms of phase-summed fluxes. Initial conditions for component α are given as

$$C_{\alpha w}(x_i, t=0) = C_{\alpha w_0}(x_i) \quad \text{on } R \text{ for } t=0 \quad [3.25a]$$

where $C_{\alpha w_0}(x_i)$ represents the initial water phase concentration of component α at location x_i . Note that the concentrations of α in all other phases are implicit in [3.25a] via the phase partition relations [3.13] or [3.17]. Boundary conditions for the phase-summed equation are stipulated by

$$C_{\alpha w}(x_i, t) = C_{\alpha w_1}(x_i, t) \quad \text{on } S_1 \text{ for } t > 0 \quad [3.25b]$$

$$\frac{\partial C_{\alpha w}}{\partial x_n} = 0 \quad \text{on } S_2 \text{ for } t > 0 \quad [3.25c]$$

$$q_{on} \Gamma_{\alpha o} C_{\alpha w}^{IIIe} = q_n^* C_{\alpha w} - D_{\alpha ij}^* \frac{\partial C_{\alpha w}}{\partial x_j} \Big/ n \quad \text{on } S_3 \text{ for } t > 0 \quad [3.25d]$$

Equation [3.25b] describes a type-1 boundary condition on boundary region S_1 with specified α -species concentration $C_{\alpha wI}(x_i, t)$ within the porous medium at the boundary. Note again that stipulation of the water phase concentration simultaneously fixes the organic liquid, gaseous and solid phase concentrations via the partition relations. Type-1 boundary conditions for transport will be used rarely since direct control-over porous media concentration seldom occurs. One case which may be relevant would be the occurrence of a source of known concentration where diffusion is the dominant transport mechanism (a type-3 condition would be used if significant convection occurred at the boundary).

Equation [3.25c] describes type-2 boundaries with zero normal concentration gradient specified on region S_2 . The zero gradient condition indicates zero normal dispersive flux at the boundary. If normal fluid velocities are nonzero, transport across the boundary will be permitted by convection. This boundary condition is commonly applied at boundaries which have fluid efflux to permit constituent transport across the boundaries. In the event that fluid fluxes are zero normal to the boundary, condition [3.25c] stipulates zero component flux. Caution needs to be exercised in applying the type-2 condition on boundaries with inward fluid velocities of uncontaminated fluid. If the concentration at the boundary is nonzero due to presence of chemical near the surface, the type-2 condition will stipulate an inward mass flux density equal to the water phase concentration at the boundary times the phase-summed velocity, q_n^* , which is incorrect. In such a case, a type-3 boundary condition with zero influent concentration should be specified to force the desired zero-flux condition. The type-2 zero gradient condition is the default condition.

Equation [3.25d] is a type-3 boundary condition for use on boundary regions, S_3 which have inward NAPL phase fluxes predicated on the assumption that contaminant enters the system solely via inflow of nonaqueous phase liquid. Here, q_{on} is the normal Darcy velocity of the oil phase at the boundary and $C_{\alpha w}^{IIIe}$ is the equivalent water phase concentration of species α in the influent oil phase defined by $C_{\alpha w}^{IIIe} = C_{\alpha o}^{III} / \Gamma_{\alpha o}$ where $C_{\alpha o}^{III}$ is the actual concentration of α in the influent oil. Note that applying the condition $C_{\alpha w}^{IIIe} = 0$ corresponds to imposing zero mass flux of component α on the boundary segment. In applying the type-3 boundary condition during periods of oil infiltration, it is important to ensure consistency in the specified oil phase concentrations such that

$$\sum_{\alpha=1}^{n_s} C_{\alpha o} = \rho_o \quad [3.26]$$

where $C_{\alpha o}$ ($\alpha=1, \dots, n_s$) is the oil phase concentration expressed as mass of component per phase volume for component α . Equivalently, in terms of mass fractions the condition may be expressed as

$$\sum_{\alpha=1}^{n_s} f_{\alpha o} = 1 \quad [3.27]$$

where $f_{\alpha o}$ is the mass fraction of component α , in the oil phase. Mass fractions and phase concentrations are related by

$$C_{\alpha p} = f_{\alpha p} \rho_p \quad [3.28]$$

where ρ_p is the bulk phase density. Simple mixing theory permits component mass fractions and volume fractions to be related as

$$\sum_{\alpha=1}^{n_s} \frac{C_{\alpha o}}{\rho_{\alpha}} = 1 \quad [3.29]$$

where ρ_{α} is the density of pure noninert components. The oil phase density may be related to phase composition by

$$\rho_o = \frac{1}{\sum_{\alpha=1}^{n_s} f_{\alpha o} / \rho_{\alpha}} \quad [3.30]$$

In applying the type-3 oil infiltration boundary condition, influent oil phase concentrations, $C_{\alpha w}^{IIIe}$ must be specified such that [3.26] - [3.30] are obeyed.

3.2 Numerical Model Description

3.2.1 General solution approach

Fluid flow equations are highly coupled with each other due to interdependence of fluid permeabilities, saturations and pressures mandating a simultaneous solution approach as discussed in the previous chapter. The flow equations are also coupled with the transport equations via the occurrence of interphase mass transfer terms and through the dependence of

various coefficients in the flow equations on fluid composition—e.g., phase density, viscosity, scaling factors, etc. Since mass transfer rates are necessarily small for the case of low solubility organic fluids and changes in fluid properties over short time periods will accordingly also be small, the dependence of the flow equations on transport will be very mild over short time spans permitting computational decoupling. Over extended periods of time, cumulative phase mass transfer may have significant effects on flow as dissolution and volatilization deplete the nonaqueous phase liquid requiring some means of updating phase transfer rates as well as compositionally sensitive fluid properties. MOTRANS considers fluid compositional effects on phase density but disregards effects on other coefficients. Interphase mass transfer rates and phase densities are time-lagged in the flow solution and updated at the end of each time-step after solution of the transport equations.

The transport equations are highly dependent on the solution of the flow equations due to the occurrence of fluid velocity and phase saturation terms directly in the transport equations and in the functional forms for the dispersion coefficients. Thus, the flow equations must be solved concurrently with or prior to evaluating transport. Due to the weak back-coupling, the most opportunistic approach is to solve the transport-equations serially with the flow equations. Furthermore, since the individual component transport equations are weakly coupled with each other in the present model due to the assumption that components do not interact, the transport equations for different components may be solved serially in arbitrary sequence.

The solution approach for solving the coupled multiphase flow and multicomponent transport problem when equilibrium mass transfer is assumed is as follows:

1. Solve the fluid flow equations simultaneously for the current time-step using time-lagged phase densities and interphase mass transfer rates.
2. Solve the phase-summed transport equation using the previous time-step phase densities and interphase mass transfer rates.
3. Back-calculate new interphase mass transfer rates and update phase densities for the current time step.
4. Proceed to the next time step.

When nonequilibrium mass transfer is considered, a modified solution approach is employed as follows:

1. Solve the fluid flow equations simultaneously for the current time-step using time-lagged phase densities and interphase mass transfer rates.
2. Solve the phase-summed transport equation using current values of apparent partition coefficients, interphase mass transfer rates and phase densities.

3. Back-calculate interphase mass transfer rates, update phase densities and apparent partition coefficients and repeat (2) until transport solution converges.
4. Proceed to the next time step.

3.2.2 Finite element formulation

The phase-summed transport equations given by [3.15] or [3.16] are solved using an upstream-weighted Galerkin finite element method with linear rectangular elements. We will present the solution for [3.15]. The formulation in terms of [3.16] is fundamentally identical. Employing linear shape functions, N_I , the concentration $C_{\alpha w}(x_i, t)$ can be approximated by

$$C_{\alpha w}(x_i, t) = \sum_{J=1}^4 N_J(\epsilon, \eta) C_{\alpha w J}(t) \quad [3.31]$$

where $C_{\alpha w J}$ denotes the concentration at node J and ϵ and η are local coordinates. Detailed information pertaining to the upstream weighting functions have been discussed by *Kaluarachchi and Parker* (1989). The Galerkin finite element approximation of [3.15] over the entire domain R can be written as

$$\int_R N_I L(C_{\alpha w}) dR = 0 \quad [3.32]$$

where $L(C_{\alpha w})$ is an operator for the phase-summed transport equations. A set of equations results of the form

$$[P] \{C_{\alpha w}\} + [M] \left\{ \frac{d C_{\alpha w}}{d t} \right\} = \{R\} \quad [3.33]$$

Using the type-3 boundary condition given by [3.25d] and disregarding cross derivative terms, the matrices $[P]$, $[M]$ and $\{R\}$ are defined by

$$\begin{aligned} P_{IJ} = & \sum_{e=1}^N \int_{R_e} D_{\alpha i i}^* \frac{\partial W_I}{\partial x_i} \frac{\partial N_J}{\partial x_i} dR + \sum_{e=1}^N \int_{R_e} W_I q_{\alpha i}^* \frac{\partial N_J}{\partial x_i} dR \\ & + \sum_{e=1}^N \int_{R_e} N_I \mu_{\alpha}^* N_J dR - \sum_{e=1}^{N_s} \langle q_n^* \rangle \int_{S_e} W_I N_J dS \end{aligned} \quad [3.34a]$$

$$M_{IJ} = \sum_{e=1}^N \int_{R_e} N_I \phi_{\alpha}^* N_J dR \quad [3.34b]$$

$$R_I = - \sum_{e=1}^{N_s} \langle q_{on} \rangle \Gamma_{\alpha o} C_{\alpha w}^{IIIe} \int_{S_e} W_I dS \quad [3.34c]$$

where N is the total number of elements, N_s is the total number of boundary elements, W_I is the asymmetric upstream weighting function, $\langle q_{on} \rangle$ is the average normal oil flux along the surface S where contaminant enters the system and $\langle q_n^* \rangle$ is the average normal phase-summed velocity on surface S . If an evaporative boundary is present, the term $\langle q_n^* \rangle$ in [3.34c] will have an additional term $(-D_{\alpha a}^{dif} \Gamma_{\alpha a})$ to account for the atmospheric boundary layer and the terms containing $C_{\alpha w}^{IIIe}$ in [3.34c] will vanish.

Treatment of the integrals in [3.34] employs the method of influence coefficients described in the flow analysis and will not be repeated here. Handling of the convective term in [3.34a] using the influence coefficient method has not been previously described and will be discussed below. Phase-summed velocities within an element are represented by

$$q_{\alpha i}^* (x_i, t) = \sum_{g=1}^4 N_g(\xi, \eta) q_{\alpha i g}^*(t) \quad [3.35]$$

where $q_{\alpha i g}^*$ is the phase-summed velocity at the evaluation points in the element, which may be at the nodes, at Gauss points or elsewhere as controlled by the parameter GP (see discussion in flow analysis). Using equation [3.35] on the convective term of [3.34a] and using linear upstream weighting shape functions (*Kaluarachchi and Parker, 1989*), it is possible to show that

$$\sum_{e=1}^N \int_{R_e} W_I q_{\alpha i g}^* \frac{\partial N_J}{\partial x_i} dR = \sum_{e=1}^N \sum_{g=1}^4 \left(\frac{m}{2} \{ [H^{xu}]_g + [H^{xg}]_g \} + \frac{d}{2} \{ [H^{yu}]_g + [H^{yg}]_g \} \right) \quad [3.36]$$

where m and d are the width and height of a rectangular element, x and y are the coordinate axes and matrices $[H]$ with superscripts xg and yg refer to the contributions from standard linear shape functions while matrices with superscripts xu and yu refer to contributions from upstream weighting coefficients. Details of matrices $[H]$ are described in detail by *Kaluarachchi and Parker (1989)* and will not be repeated here. The surface integrals in [3.34a] and [3.34c] can be

described by

$$\begin{aligned} \int_{S_e} W_I N_J dS &= \frac{\ell}{12} (4 \pm 3\omega) & \text{if } I = J \\ &= \frac{\ell}{12} (2 \pm 3\omega) & \text{if } I \neq J \end{aligned} \quad [3.37a]$$

and

$$\int_{S_e} W_I dS = \frac{\ell}{2} (1 \pm \omega) \quad [3.37b]$$

where ℓ is the length of the side and ω is the upstream weighting coefficient. The appropriate sign of the integrals given in [3.37] will be determined by the side of the element exposed to the boundary condition.

Time integration of [3.33] is performed using a standard finite difference approximation. The resulting final set of equations can be written as

$$\left(\theta [P] + \frac{[M]}{\Delta t_{k+1}} \right)^{k+1} \{C_{\alpha w}\}^{k+1} = \left(\frac{[M]}{\Delta t_{k+1}} + (\theta - 1) [P] \right)^k \{C_{\alpha w}\}^k + \{R\}^{k+\theta} \quad [3.38]$$

where k and $k+1$ refer to previous and current time steps and θ is a time weighting factor where $0.5 \leq \theta \leq 1$ for an unconditionally stable temporal approximation. Time-step size is varied under program control by a time incremental factor which increases or decreases time-step size depending on the number of iterations required-for solution of the flow problem. The time-step size for solution of the transport problem is taken as identical to that for the flow problem. If equilibrium mass transfer is assumed, the transport equation is linear and no iteration of the solution is required. For the case of nonequilibrium mass transfer, nonlinearities are handled by a simple Picard iteration scheme with apparent partition coefficients, mass transfer rates and phase densities updated at each iteration. The convergence criterion for the aqueous concentration ($C_{\alpha w}$) of species α is as follows

$$|C_{\alpha w}^{r+1} - C_{\alpha w}^r| \leq |C_{\alpha w}^r| e_r + e_\alpha \quad [3.39]$$

where $r+1$ and r refer to current and previous iterations, e_r is the allowable relative convergence error which is internally set equal to 0.001 and e_α is the allowable absolute convergence error for species α . This convergence criteria must be met at all nodes.

3.2.3 Interphase mass transfer and density updating

After solution of the phase-summed transport equations, the interphase mass transfer terms R_{ap} must be updated. This is performed after each iteration of the transport equations in the case of nonequilibrium mass transfer. For the equilibrium case, the transport model is linear and no iteration is required. Hence, for the latter case, updating is performed only once at the end of each time step. To compute the mass transfer rates, the concentrations of each component in the oil, gas and solid phases are first calculated from the partition coefficients (eq. 3.13 for the equilibrium case or 3.17 for the nonequilibrium case) and from the control phase concentrations (C_{aw} for the case of eq. 3.15 or C_{aw} for eq. 3.16). The mass transfer rate terms, R_{ap} , are computed by back-substitution into the component transport equations for each phase (eqs. 3.11 and 3.12) using a finite difference approximation. Summing over the components yields the desired R_p terms for each phase for use in the subsequent solution of the flow and phase-summed transport equations.

For equilibrium mass transfer problems, effects of mass transfer terms on the flow and transport equation solutions at any given time-step will be quite small. However, cumulative effects can be very important since these terms will control the long term removal of NAPL associated with dissolution and/or volatilization. The accuracy of interphase mass transfer calculations will generally be most, troublesome during periods of highly transient NAPL flow. During such periods, it may be preferable to suppress mass transfer updating to avoid numerical instability as well as to reduce computational effort and improve accuracy. Therefore, MOTRANS provides the user with the option of performing interphase mass transfer calculations at each time-step or of not performing such calculations. This option can be used when equilibrium mass transfer is assumed.

With increasing simulation time, the density of each phase will change depending on the net mass of each component leaving or entering the phase. Although density derivatives were neglected in the equation development, on the assumption that these terms are small over a given time step, cumulative changes in density cannot be ignored since over long times these can accumulate and become quite large in magnitude. To accommodate these effects, liquid phase densities are updated at the end of each time-step as follows

$$\rho_w = \rho_w^o \left[1 - \sum_{\alpha=1}^{n_s} \frac{C_{\alpha w}}{\rho_\alpha} \right] + \sum_{\alpha=1}^{n_s} C_{\alpha w} \quad [3.40a]$$

$$\rho_o = \sum_{\alpha=1}^{n_s} C_{\alpha o} \quad [3.40b]$$

where n_s denotes the number of organic species, ρ_w^o is the density of uncontaminated water, ρ_α is the density of pure α -component. Density ratios, ρ_{rw} , ρ_{ro} and ρ_{ra} , are computed as the ratio of ρ_w , ρ_o and ρ_a to ρ_w^o .

For the gas phase, density depends on both pressure and composition. Pressure dependence is treated as a nonlinear effect in the gas flow equation according to

$$\rho_a = \lambda h_a + \rho_a^o + \rho_a^c \quad [3.41]$$

where λ is the gas compressibility taken to be $1.17 \times 10^{-6} \text{ g cm}^{-4}$, ρ_a^o is the density of native soil air taken to be $1.12 \times 10^{-3} \text{ g cm}^{-3}$, and ρ_a^c is the density of contaminants in the gas phase computed as

$$\rho_a^c = \sum_{\alpha=1}^{n_s} C_{\alpha a} \quad [3.42]$$

where $C_{\alpha a}$ is the gas phase concentration of species α and n_s is the number of noninert organic species.

In certain problems, numerical oscillations may lead to unacceptable mass balance error in the bulk fluid phases on in the components. A mass injection scheme has been implemented in the code that distributes mass balance errors within the system. If this option is invoked and flow only is being analyzed, the volumetric error for the oil phase (net change within domain minus boundary fluxes) is computed at the end of each time step, and the error is reinjected during the next time step in proportion to the local oil phase saturation. If flow and transport is analyzed, the mass balance error for each component is computed at the end of each time step, taking into account boundary fluxes of the components in water, oil and gas phases; and the error is reinjected during the nest time step in proportion to the local oil phase saturation.

4. GUIDE TO USE OF MOTRANS

4.1 Estimation of Soil and Fluid Properties

4.1.1 Soil properties

Soil properties required for analyses of multiphase flow using MOTRANS include the saturated conductivity to water in the vertical direction, K_{sw} , and the horizontal direction, K_{sh} , soil porosity, ϕ , apparent irreducible water saturation, S_m , maximum residual oil saturation for water imbibition, S_{or}^{max} , and the van Genuchten air-water capillary retention parameters, α and n . Typical values for the maximum residual oil saturation, S_{or}^{max} , are in the range of 0.15-0.35. Values tend to increase for more heterogeneous porous materials and may be dependent to a certain extent on fluid properties with higher viscosity fluids tending to have larger residual saturations. Estimation of van Genuchten parameters from grain size distribution data (*e.g.*, Mishra *et al.*, 1989) can provide parameters which are fairly reliable, although analyses on laboratory core samples are desirable for more accurate determinations. Estimates of hydraulic conductivities can also be inferred from grain size distribution data, but are subject to large uncertainty. Therefore, field or laboratory measurements to determine hydraulic conductivity is always desirable. Typical values of capillary pressure curve parameters and vertical hydraulic conductivities are tabulated in Table 4.1 for a variety of soil types. Horizontal conductivities are commonly 2-5 times higher than vertical conductivities. From Table 4.1 it is observed that ranges of ϕ , S_m and n are quite narrow compared to α and K_{sw} . Furthermore, a useful-correlation between the latter variables may be noted as

$$\alpha \approx \left(K_{sw} / A \right)^{1/2} \quad [4.1]$$

where $A=0.5 \text{ m}^3 \text{ d}^{-1}$ ($\pm 50\%$) which provides a *rough* estimate of α if field data on the hydraulic conductivity are available.

To model chemical transport, two additional porous medium parameters are required by MOTRANS for the case of equilibrium phase transfer. These are the longitudinal and transverse dispersivities, A_L and A_T . MOTRANS assumes that these parameters may be regarded as porous media properties which are constants for all phases and independent of phase saturation or composition. It is known that dispersivity for nonreactive chemical transport is controlled largely by porous media heterogeneity which typically increases with the scale of observation such that A_L typically is on the order of 1-10% of the scale of the maximum plume dimension and A_T is several times smaller than A_L .

When consideration is given to nonequilibrium phase partitioning during transport, the nonequilibrium coefficients, k_{oa} , k_{wa} , k_{ow} , and k_{ws} , must be specified. At the present time, little practical guidance can be given regarding the specification of these parameters. A few recent

laboratory studies have been reported which deal with this problem suggesting that rate constants for homogeneous soil columns are sufficiently large to yield near-equilibrium fluid-fluid interphase mass transfer unless velocities are unusually high. However, information on the effects of heterogeneity at the field scale on mass partitioning is virtually nonexistent. Since the time scale for mass transfer between zones of differing hydraulic properties is much greater than the time scale for pore scale mass transfer, the former may be expected to have a greater impact on field behavior. Given site measurements of contaminant concentrations, mass transfer coefficients may be estimated by "history matching." A better understanding of mass transfer kinetics at the field scale awaits future study.

Table 4.1 Typical soil properties for various soil types.

Soil type	K_{sz} [m/d]	ϕ [-]	S_m [-]	α [m ⁻¹]	n [-]
Sand	7.1	0.43	0.09	14.5	2.7
Loamy sand	3.5	0.41	0.15	12.4	2.3
Sandy loam	1.06	0.41	0.15	7.50	1.9
Sandy cl. loam	0.31	0.39	0.26	5.9	1.5
Loam	0.25	0.43	0.19	3.6	1.6
Silty loam	0.11	0.45	0.16	2.0	1.4
Clay loam	0.062	0.41	0.22	1.9	1.3
Silt	0.060	0.43	0.07	1.6	1.4
Sandy clay	0.029	0.38	0.26	2.7	1.2
Silty cl. loam	0.017	0.43	0.21	1.0	1.2
Silty clay	0.0048	0.36	0.19	0.5	1.1

4.1.2 Bulk fluid properties

Bulk fluid properties which are required to model multiphase flow are the scaling coefficients, β_{ao} and β_{ow} and specific gravities and relative viscosities of the NAPL and gas phases if considered in the flow analysis. If coupled flow and transport analyses are performed, the program will compute the phase specific gravities internally as a function of the current phase compositions. If analyses of flow-only are performed, the user must input the specific gravity of NAPL, ρ_{ro} . If gas flow is considered, the program assumes a specific gravity of air at atmospheric pressure of 0.0012 and an air-water viscosity ratio of 0.018. If the NAPL specific gravity is not known from measurements, but the composition is known, the oil specific density may be computed as

$$\rho_{ro} = \frac{1}{\sum_{\alpha} f_{\alpha o} / \rho_{r\alpha}} \quad [4.2]$$

where $f_{\alpha o}$ is the mass fraction in the oil phase of organic component α and $\rho_{r\alpha}$ is the specific gravity of component α .

Although NAPL viscosity varies with fluid composition, MOTRANS assumes these effects are comparatively minor and does not update viscosity for temporal phase composition changes. Bulk phase viscosity may be determined experimentally for the fluid of concern, or an estimate may be made from the phase composition if this is known via

$$\eta_{ro} = \sum_{\alpha} f_{\alpha o} \eta_{r\alpha} \quad [4.3]$$

where $\eta_{r\alpha}$ is the relative viscosity of component α .

Capillary pressure curve scaling parameters may be estimated from surface tension and interfacial tension data via

$$\beta_{ao} = \frac{\sigma_w}{\sigma_o} \quad [4.4a]$$

$$\beta_{ow} = \frac{\sigma_w}{\sigma_{ow}} \quad [4.4b]$$

where σ_w is the surface tension of pure water (i.e., 72 dynes/cm), σ_o is the surface tension of the NAPL and σ_{ow} is the interfacial tension between NAPL and water.

Surface and interfacial tensions of mixtures may be measured directly or estimated from the NAPL composition via

$$\sigma_o = \sum_{\alpha} f_{\alpha o} \sigma_{\alpha} \quad [4.5a]$$

$$\sigma_{ow} = \sum_{\alpha} f_{\alpha o} \sigma_{\alpha w} \quad [4.5b]$$

where σ_α is the surface tension of pure α component, $\sigma_{\alpha o}$ is the interfacial tension of α with water, and $f_{\alpha o}$ is the mass fraction of α in the NAPL. In the absence of interfacial tension data, an estimate of β_{ow} may be made from the relation

$$\beta_{ao} = \frac{1}{1 - \frac{1}{\beta_{ow}}} \quad [4.6]$$

Furthermore, since numerical difficulties can be induced when deviation from [4.6] occur during the transition from an air-water to an air-oil-water system, it is recommended to employ scaling factors which *force* condition [4.6]. If β_{ao} and β_{ow} are estimated from [4.4] and condition [4.6] is not met, the condition may be imposed by the following means

$$\beta'_{ao} = f^{cor} \beta_{ao} \quad [4.7a]$$

$$\beta'_{ow} = f^{cor} \beta_{ow} \quad [4.7b]$$

where

$$f^{cor} = \frac{1}{\beta_{ao}} + \frac{1}{\beta_{ow}} \quad [4.7c]$$

in which β'_{ao} and β'_{ow} are "corrected" parameter values which may be used in lieu of β_{ao} and β_{ow} values which are computed directly from [4.4]. For hydrocarbons which have low solubility in water, condition [4.6] is generally closely approximated. For gasoline, the values β'_{ao} and β'_{ow} estimated from surface tension data are 3.2 and 1.45, respectively ($\pm 10\%$).

Another empirical method for estimating scaling coefficients, based on a correlation developed for crude oil surface tension, is

$$\beta_{ao} = 2 \rho_{ro} \quad [4.8a]$$

$$\beta_{ow} = \frac{1}{1 - \frac{0.5}{\rho_{ro}}} \quad [4.8b]$$

where ρ_{ro} is the specific gravity of the NAPL. Values of surface tensions, interfacial tensions, specific gravities and relative viscosities for a number of common hydrocarbon compounds which occur in groundwater are tabulated in Table 4.2.

4.1.3 Component properties

In order to model component transport, a number of additional physical and chemical properties of the NAPL components must be known. These include the diffusion coefficients in bulk water, oil and air ($D_{\alpha w}^o$, $D_{\alpha o}^o$ and $D_{\alpha a}^o$), the oil-water, air-water and solid-water partition coefficients ($\Gamma_{\alpha o}$, $\Gamma_{\alpha a}$ and $\Gamma_{\alpha s}$) and the first-order decay coefficients ($\mu_{\alpha w}$, $\mu_{\alpha o}$, $\mu_{\alpha a}$ and $\mu_{\alpha s}$). Molecular diffusion coefficients in bulk water and air can be found tabulated for many common industrial chemicals or they may be estimated using semi-empirical estimation methods (see *Lyman et al.*, 1982). Oil phase diffusion coefficients can be estimated from the water phase diffusion coefficient by the empirical relation

$$D_{\alpha o}^o = \frac{D_{\alpha w}^o}{\eta_{ro}} \quad [4.9]$$

where η_{ro} is the relative viscosity of the bulk oil phase.

The equilibrium partition coefficient between air and water is commonly referred to as Henry's constant. The form employed here is the dimensionless form of Henry's law. In some references, the user may find tabulated data for Henry's law in terms of gas partial pressures rather than concentrations which leads to Henry's constants with units of pressure x length x mass⁻¹. To obtain the dimensionless Henry's constant, $\Gamma_{\alpha a}$, from the pressure form, H_{α} , the relationship to employ is

$$\Gamma_{\alpha a} = H_{\alpha} M_{\alpha} / R T \quad [4.10]$$

where M_{α} is the molecular weight of species α , R is the ideal gas constant and T is the absolute temperature. In the absence of measured data, various estimation methods may be employed to estimate Henry's constants (*Lyman et al.*, 1982).

The oil-water partition coefficient, $\Gamma_{\alpha o}$ is commonly referred to as Raoult's constant. For low solubility organics which are liquids at normal temperatures, an estimate of this coefficient may be obtained from the aqueous solubility and pure phase density as

$$\Gamma_{\alpha o} = \rho_{\alpha} / C_{\alpha w}^o \quad [4.11]$$

where ρ_{α} is the density of pure α and $C_{\alpha w}^o$ is the aqueous solubility.

Estimation of solid phase partition coefficients for hydrophobic organic compounds may be performed in various ways. First, it should be noted that the dimensionless coefficient $\Gamma_{\alpha s}$ is

related the commonly used "distribution coefficient", k_d , via

$$\Gamma_{\alpha s} = \rho_b k_{d\alpha} \quad [4.12]$$

where ρ_b is the porous medium bulk density. Adsorption coefficients for hydrophobic organics are often estimated using a correlation with organic carbon content which gives

$$\Gamma_{\alpha s} = \rho_b f_{oc} k_{oc\alpha} \quad [4.13]$$

where f_{oc} is the organic carbon mass fraction in the soil and $k_{oc\alpha}$ is the organic carbon normalized adsorption coefficient which may be estimated from solubility or from chemical structure by various means (*e.g.*, Lyman *et al.*, 1982).

The estimation of first-order decay coefficients ($\mu_{\alpha w}$, $\mu_{\alpha o}$, $\mu_{\alpha a}$, and $\mu_{\alpha s}$) is more problematic due to their nebulous physical significance. True first-order chemical decomposition will occur due to hydrolysis reactions which can have rate constant which can be found tabulated for many common compounds. However, biologically mediated transformations are generally much more significant processes in the field and the corresponding apparent rate coefficients are dependent on a large number of environmental variables. Since decay may be expected to occur nearly exclusively within the aqueous phase, ignoring all terms except $\mu_{\alpha w}$ is probably justified. Existing field and laboratory studies on the chemicals of concern under similar conditions may be used to estimate the desired rate coefficients. However, it should be recognized that without calibration at the site under consideration, the estimated rate coefficients will be subject to considerable uncertainty.

A list of physical and chemical properties of selected organic compounds of environmental significance is given in Table 4.2.

Table 4.2 PROPERTIES OF ORGANIC COMPOUNDS AT 20° C

Organic compound	Diff.coef. in water (m ² /d)	Diff. coef. in air (m ² /d)	Relative viscosity (-)	Specific gravity (-)	Surface tension (dyne/cm)	Interfacial tension (dyne/cm)	Henry's constant (-)	Water solubility (g/m ³)
Benzene	9.42x10 ⁻⁵	0.76	0.65	0.878	27.90	28.88	2.40E-01	1780.0
Toluene	8.21x10 ⁻⁵	0.68	0.58	0.867	29.00	36.10	2.80E-01	515.0
o-xylene	6.21x10 ⁻⁵	0.61	0.81	0.880	31.21	36.06	2.20E-01	152.0
Ethylbenzene	6.21x10 ⁻⁵	0.61	0.68	0.867	29.20	35.48	3.70E-01	152.0
Trichloroethylene	7.28x10 ⁻⁵	0.71	0.59	1.464	29.30	34.50	4.20E-01	1100.0
Tetrachloroethylene	6.56x10 ⁻⁵	0.64	0.90	1.623	31.30	44.40	3.50E-01	150.0
1,1,1 Trichloroethane	7.01x10 ⁻⁵	0.69	1.20	1.339	25.40	45.00	7.70E-01	4400.0
1,1 Dichloroethane	7.89x10 ⁻⁵	0.78	0.44	1.176	24.66	47.20	2.40E-01	5500.0
1,3 Dichlorobenzene	6.28x10 ⁻⁵	0.62	1.48	1.288	37.00	40.00	1.10E-01	111.0
Carbon Tetrachloride	7.05x10 ⁻⁵	0.70	0.97	1.594	27.00	45.00	9.70E-01	800.0
1,2,4 Trichlorobenzene	5.93x10 ⁻⁵	0.57	2.77	1.454	45.57	27.13	4.30E-02	4.8

4.2 Program Structure and Operation

4.2.1 *Basic features and program control*

4.2.1.1 Basic problem definition. MOTRANS may be used to analyze flow problems involving two phase oil-water flow with gas at atmospheric pressure (IOIL=1, IAIR=0) or two phase air-water including explicit consideration of gas flow (IOIL=0, IAIR=1) or three phase air-oil-water flow (IOIL=1, IAIR=1). Problems involving flow only may be analyzed (ITRN=0) or coupled flow and transport may be modeled (ITRN=1) for NAPLs containing up to 5 partitionable species (NTSP). Problems may be run for plane sections (IRAD=0) or in radially symmetric sections (IRAD=1).

4.2.1.2 I/O unit numbers used by program. MOTRANS uses five unit numbers for data input and output designated internally as NR, NO, NINP, and NOUT (units 5, 6, 8, and 9 respectively). NR and NO correspond to main input and output files. NOUT is an auxiliary output unit to dump results of the last converged time-step for restarting purposes. NINP is the unit number for the auxiliary input data file for restarting which is identical to the file dumped by NOUT from the previous simulation. In addition, a number of files in unformatted structure for internal storage are used corresponding to units NWK1, NWK2 and NTRD. If the restart option is used, the auxiliary data file must exist to define the initial conditions for the entire problem including gas convection and transport if required. The parameter TIME for the restart problem would normally be adjusted to correspond to the ending time of the previous simulation.

4.2.1.3 Use of consistent units. Linear dimensions can be in centimeters or meters depending on the value of IDIM and any consistent units for time may be employed. For analyses involving transport, units of mass may be in milligrams, grams or kilograms depending on the value of KUNIT. Units of input parameters are indicated in Appendix A and should be adhered to religiously! Units are specified generically as L=length, M=mass and T=time. Units of dimensionless variables are denoted by [-]. When consideration is given to integrated fluxes across boundary regions, it should be kept in mind that boundary integrals from plane slice problems will yield quantities per unit width in the direction perpendicular to the plane of the problem, whereas radial problems are already integrated in the radial direction.

4.2.1.4 Maximum array dimensions. The program is dimensioned to accommodate problems with up to 1500 nodes with rectangular meshes up to 50 nodes in width or height. The porous medium may consist of up to 10 different soil types. For the main flow module, up to 100 type-1 and 100 type-2 boundary nodes or element sides may be specified for each phase described by up to 100 schedules with up to 4 subschedules per schedule allowed. The transport module can accommodate up to 5 non-inert species with a total of 100 type-1 and 100 type-3 boundary nodes or element sides for each species. Transport boundaries may be described by up to 100 schedules with as many as 4 subschedules per schedule.

4.2.1.5 Program control and termination. When data files are first prepared or after significant changes have been made, it is desirable to verify that the input is correct by first reading the data file and echoing it back. This may be done by setting the parameter IRUN=0 which will echo

input data as well as print out information on initial conditions at all nodes. It is recommended to always use this before running a problem. Having verified the input data to this extent, it is suggested to first run only a few time steps to check whether convergence behavior and accuracy (e.g., mass balance) are acceptable. Termination can be controlled for such purposes by stipulating appropriate values of the maximum number of time-steps (MXTST) or the maximum simulation time (TMAX). Normal program termination will occur if one of several criteria are met:

- (1) Current time of simulation exceeds input value of TMAX
- (2) Total number of time steps exceeds input value of MXTST
- (3) Change in NAPL volume in system exceeds input value of TINF if JINF=1
- (4) Change in water volume in system exceeds input value of TINF if JINF=2
- (5) Change in gas volume in system exceeds input value of TINF if JINF=3

4.2.1.6 Convergence and time-step control. For a given phase p , the allowable convergence error ϵ_i at node i for the solution of the nonlinear flow equations is given by

$$\epsilon_i = h_{pi}^r \epsilon_r + \epsilon_a \quad [4.14a]$$

and all nodes must satisfy the condition

$$| h_{pi}^{r+1} - h_{pi}^r | \leq \epsilon_i \quad [4.14b]$$

where h_{pi}^r and h_{pi}^{r+1} are p -phase heads at node i for the current and previous iterations, ϵ_r is the prescribed relative convergence error (RCON) and ϵ_a is the prescribed absolute convergence error (ABSA). Termination occurs if convergence is not met in MCNT iterations. If convergence occurs in more than MCNT/3 iterations, the simulation will proceed to the next time-step but reduce the time-step size by a factor TFACT. If the solution converges in less than or equal to MCNT/4 iterations, the time-step size for the subsequent time-step will be increased by a factor of TFACT which should range between 1.01 and 1.05.

If termination occurs due to nonconvergence, the user has a number of options since many factors influence convergence behavior. Some steps which may be taken to remedy nonconvergence are: reduce the initial time-step size (DELTA) and the timestep increment factor (TFACT), increase the upstream weighting factor for the flow problem (UFW), switch off interphase mass transfer during highly transient flow periods (KUDAT=0), apply changes in boundary conditions gradually using "ramping" as described later, relax the relative or absolute convergence criteria (RCON and ABSA), make the mesh finer, reduce the size of the domain, or run the problem in stages with output from early stages used to define later stages.

If nonequilibrium interphase mass transfer is modeled, the transport equation is solved iteratively using a Picard scheme with convergence criteria defined by

$$e_i = C_{\alpha w i}^r e_r + e_\alpha \quad [4.15]$$

where $C_{\alpha w i}^r$ is the water phase concentration at node i for the previous iteration, e_r is a relative convergence criterion which is internally set to 0.001, and e_α is the user-specified absolute convergence criterion for species α in the water phase.

4.2.1.7 Upstream weighting. Upstream-weighting is a useful technique to reduce the nonlinearity of the multiphase flow equations and obtain a more stable solution of the transport equations free of oscillations. In selecting suitable values for upstream-weights, it is preferable to use the minimum value necessary to obtain convergence since high values may result in numerical dispersion at sharp fronts especially in the transport solution. Upstream-weights may range from 0 to 1 with 0 representing no upstream-weighting and 1 corresponding to full upstream-weighting. Values around 0.5 may be selected to start a problem and these may be adjusted upward if oscillations in the solutions occur. A few preliminary runs may be used to evaluate the sensitivity of the results to the upstream weights for the flow equations (UFW) and for transport (UFT).

4.2.1.8 Automatic control of oil and water flow solutions. MOTRANS provides two options for controlling the oil and water flow equation solutions to reduce computational effort. In many problems, oil saturations in the domain may reach residual levels after which they do not change with time (except due to interphase mass transfer). If changes in oil saturation at every point in the domain are less than a specified tolerance (TOL3) over a time-step, MOTRANS will not solve the oil flow equation for subsequent timesteps. That is, the system will be regarded as an air-water system with oil in a residual occluded state. Oil saturation is updated after subsequent time-steps to account for mass lost due to dissolution and volatilization if the transport equation is being solved. This option is invoked by setting KFEMC=1 and specifying TOL3 > 0. If KFEMC=1 the oil equation to be solved at all times. Using TOL3 of 0.0001 to 0.001 is satisfactory for most problems. *Caution:* Once the oil equation is switched off, it cannot be reactivated unless the problem is restarted. If time-varying boundary conditions are such that oil may become trapped (e.g., rising water table) and later released (e.g., falling water table), the user should be careful of using TOL3.

The second method of controlling the liquid flow equations uses the ASD method. In this method, elements are categorized as "active" or "inactive" at a given iteration. If the element is active, then it is included in the global matrix assembly, otherwise it is excluded. The criteria for changing a node from inactive to active is based on the changes in water pressure head, oil pressure head, oil saturation, and water saturation at connected nodes from the last converged time-step to the current iteration. The specific criteria for changing an element from inactive to active is

$$\begin{aligned}
& \Delta h_w > TOL1 \\
& \text{or} \\
& \Delta h_o > TOL1 \\
& \text{or} \\
& \Delta S_w > TOL2 \\
& \text{or} \\
& \Delta S_o > TOL2
\end{aligned}$$

where Δh_w , Δh_o , ΔS_w , and ΔS_o are the changes in h_w , h_o , S_w , and S_o , respectively, between the previous converged time-step and the current iteration, TOL1 is a specified head tolerance and TOL2 is a specified saturation tolerance. Equations for nodes on the active-inactive frontier will have contributions only from active elements and the boundary will shift naturally as imbibition or drainage "fronts" pass through the domain. To enable the ASD option, the switch IFEMC must be set to 0 and TOL1 and TOL2 set to appropriate values. Values for TOL1 of 0.0001 to 0.0001 m and for TOL2 of 0.0001 to 0.001 are generally applicable for most problems.

4.2.1.9 Automatic control of gas flow solution. MOTRANS provides a number of features to control the gas flow solution which enable gas flow to be considered while minimizing the computational effort and improving solution robustness. The user has the option of disregarding gas compressibility (ICOM=0) which reduces the degree of nonlinearity of the gas flow solution. If gas pressure-differences in the domain are within a few tenths of atmospheres, or if the transient behavior of the gas flow solution is not of concern, this option may be invoked.

In many problems of practical interest, gas withdrawal or injection at constant pressure is imposed which will result in a steady state flow problem after some time. To minimize unnecessary computational effort, the user can specify a tolerance for eliminating the gas flow equations from the flow solution when the gas pressures approach steady state. If changes in gas heads for all nodes in the domain are less than TMXG over a time step, gas flow will be assumed steady and the gas equation will not be solved for subsequent time steps (LAIR is internally set to 0). If ITRN=1, gas velocities in the transport equation will be fixed thereafter at the steady-state values. TMXG=0 forces continuous solution of gas flow equation.

Many gas flow problems involve domains which have large portions where the gas saturation is zero (e.g., nodes below the water table). At such nodes; gas pressure has no physical meaning. Solution for gas pressure at these nodes expends fruitless effort and, more importantly, can result in a destabilizing effect on the entire solution due to the ill-defined nature of the gas flow equation at locations where gas permeability is zero. If $S_i = 1$ at a node, the program will internally fix the gas pressure head to eliminate the node from the solution domain for the gas equation.

4.2.1.10 Mass transfer updating for transport solution. Flow and transport equations are coupled through the interphase mass transfer terms, which are updated at the end of each time step and time-lagged. Phase densities are updated at this time also and lagged. During periods of highly transient flow, particularly during periods of high oil phase velocities, this decoupled approach can lead to instabilities if errors in the back-substituted mass transfer rates grow with time. Since the errors which result from disregarding interphase mass transfer over short time periods are small if the component solubilities are small, it is advisable to avoid mass transfer updating during such periods. User control over mass transfer updating is achieved through the parameter TTRN which is the simulation time at which mass transfer updating is begun. During periods of rapid oil infiltration, mass transfer updating may be entirely disabled by putting a large value for TTRN. During periods of redistribution, mass transfer updating may be disabled for the first few days. If component mass balance errors arise, it may be advisable to increase TTRN.

4.2.1.11 Mass balance correction scheme. In certain problems, numerical oscillations may lead to unacceptable mass balance error in the bulk fluid phases or in the components. An optional mass injection scheme has been implemented in the code that distributes mass balance errors within the system. If this option is invoked (IMCOR=1) and flow only is being analyzed (ITRN=0), the volumetric error for the oil phase (net change within domain minus boundary fluxes) is computed at the end of each time step, and the error is reinjected during the next time step in proportion to the local oil phase saturation. If flow and transport is analyzed (ITRN=1), the mass balance error for each component is computed at the end of each time step, taking into account boundary fluxes of the components in water, oil and gas phases, and the error is reinjected during the next time step in proportion to the local oil phase saturation.

4.2.2 Spatial discretization and mesh generation

Only rectangular elements with sides parallel to the principle axes are permitted by MOTRANS (Figure 4.1). The domain is specified to be a rectangular region. The finite element mesh is defined by the user by inputting z-coordinates of all nodes on a single vertical transect and x-coordinates (or r-coordinates) on a horizontal transect.

In order to minimize the band width of the matrices which must be solved, the global node numbering is always assumed to be in the direction of the side of the mesh with the fewest nodes, starting in the lower left hand corner. In the event of equal numbers of nodes in the vertical and horizontal directions, node numbering will be in the vertical direction by default. As an example, Figure 4.2 shows a mesh with 8 rows and 9 columns. Node numbering is thus from bottom to top as shown starting from the lower left-hand corner. Elements are numbered in the same pattern as nodes.

Figure 4.1. Local side numbering of quadrilateral elements.

Figure 4.2. Finite element mesh with numbers in parentheses indicating global element numbers and others referring to global node numbers.

It is very important to understand the global node and element numbering in order to define the boundary conditions. For flux-type boundary conditions, it is also necessary to stipulate the local element side number subjected to a prescribed flux. Local side numbering is always counterclockwise from the bottom as illustrated in Figure 4.1.

When creating a mesh, several factors should be kept in mind. The mesh should be designed so that the "aspect ratio," which is the ratio of maximum to minimum element side length, is not too great. Generally, aspect ratios should be less than 5. The mesh should be finest near locations where nonlinear boundary conditions will be most severe (e.g., boundaries with oil infiltration, gas vacuum extraction, etc.). Variations in element dimensions should not occur too abruptly in the mesh. It is recommended that changes in mesh spacing between adjacent elements are not greater than 50%.

4.2.3 Specification of initial conditions

4.2.3.1 Initial conditions for flow. Initial conditions for the flow equations involve stipulation of fluid pressure heads at all nodes in the domain. Initial conditions may be specified by the user in the main data file or may be read in from an auxiliary file for restart problems. For non-restart problems (IRES=0), initial liquid heads may be stipulated using a bilinear interpolation algorithm with heads defined on the left and right boundaries of the domain according to the relations

$$h_w = a + b z \quad [4.16]$$

$$h_o = c + d z \quad [4.17]$$

where z is the elevation along the vertical transect on the boundary and a , b , c and d are input parameters. For equilibrium conditions $a = z_{aw}$, $b = -1$, $c = \rho_{ro} z_{ao}$ and $d = -\rho_{ro}$ where z_{aw} is the air-water table elevation (elevation where $h_w = 0$) and z_{ao} is the air-oil table elevation (elevation where $h_o = 0$). When [4.16] and [4.17] are employed, values of a and c are specified on the left and right boundaries of the domain and b and d are taken as constants for the entire domain.

Note that under equilibrium conditions with zero gauge gas pressure, the air-oil elevation in an observation well corresponds to z_{ao} and $z_{aw} = z_{ao} - (1 - \rho_{ro})H_o$ where H_o is the oil thickness in the well. Forcing $H_o = 0$ will produce a no-oil condition. A "no-oil" condition will exist at a node if

$$h_o \leq \frac{\beta_{ow} h_w + \beta_{ao} h_a}{\beta_{ow} + \beta_{ao}} \quad [4.18]$$

which corresponds to the condition IUFO = 1 in the data file. In this case, c and d need not be entered and the program will assign oil heads given by equation [4.18].

MOTRANS provides the capability to restart a problem from the final time output of a previous run. During normal program termination, MOTRANS writes final phase pressures and historical information needed by the fluid entrapment model to an auxiliary output file which can be read if the restart option is invoked. If the user specifies IRES=1, oil and water heads will be read for a two phase problem (IOIL=1, IAIR=0). For a three phase problem (IOIL=1, IAIR=1), pressures of water, oil and gas are read from the restart file if IRES=1. If the restart file contains only oil and water data from a previous run with (IAIR=0) but gas flow is to be considered for the restart problem the user may use the option IRES=2 and the code will initialize gas pressures to zero. If the problem is not a restart problem and gas flow is analyzed, MOTRANS takes the initial conditions for the gas phase to be uniform at zero gauge pressure.

4.2.3.2 Initial conditions for transport. Initial conditions for transport are stipulated in terms of the water phase concentrations of each component. Three options are provided:

- KIC=1 Species concentrations are automatically assigned initial values of zero at locations where oil saturation is zero, while at other locations the water phase concentration of each species a is assigned a default value CINIT α .
- KIC=2 Initial concentrations of all species are specified for each node in the domain in the main data file.
- KIC=3 Initial concentrations of all species are read in from a restart file which must have been dumped from an earlier run with ITRN=1.

Note that if the problem is a restart problem for flow but the earlier analysis did not consider transport, KIC=3 cannot be used but KIC=1 provides a good way to continue the simulation and take into account transport. For problems involving NAPL addition over a relatively short period followed by long term redistribution and migration, the initial stages of the problem may be analyzed without considering transport with very little loss of accuracy. This can provide savings in computational effort and more importantly may provide a more stable and well-behaved problem since the short term infiltration and transport problem is relatively difficult. Consistency between the stipulated initial water phase concentrations and the NAPL composition requires care that the conditions given by equations [3.18] - [3.22] are fully adhered to. If nonequilibrium transport is considered, nonequilibrium initial conditions for the restart problem are taken into account by reading in the apparent partition coefficients for the last computed time step in addition to the phase-summed concentration solution.

4.2.4 *Specification of boundary conditions*

4.2.4.1 Boundary conditions for flow model. In the flow module, type-1 boundary conditions may be stipulated which define phase pressure heads for specified nodes, while type-2 or fluid flux boundary conditions can be stipulated on sides of elements. To prescribe the boundary

conditions, the user must know the global node numbers to which type-1 conditions are to be applied and the global element numbers as well as local side numbers of boundary segments for type-2 conditions. Global node numbering follows the pattern illustrated in Figure 4.2 with the direction of numbering always in the direction having the smaller number of nodes. In the event of equal numbers of nodes in the vertical and horizontal direction, the node numbering will be in the vertical direction. Local element side numbering is illustrated in Figure 4.1.

For the flow problem, the user specifies the total number of nodes subjected to type-1 boundary conditions for the water, oil and gas phases (NBC(1,1), NBC(2,1) and NBC(3,1)). For each phase, a list of nodes subjected to type-1 boundary conditions is given and for each node the user indicates the number of a schedule which contains information on the time-dependent values of the boundary condition at the node. A given schedule may be used for one or many nodes (if several nodes are subject to the same boundary conditions). One list of schedules is input for the entire flow problem without reference to the phase so a given schedule number could be used for both water and oil flow if the occasion arose. For example, if water at node I and oil at node J were both to be subjected to infiltration under zero pressure with the same time-dependence, then both nodes could reference the same schedule number and the program will interpret the data in the referenced schedule to be water heads in one case and oil heads in the second case. Flux boundaries are handled in a similar manner with the total number of element sides subjected to type-2 boundary conditions for each phase defined by the variables NSS(1,1), NSS(2,1) and NSS(3,1). For each phase, a list of elements and side numbers subjected to type-2 boundary conditions is then given and the user indicates the number of a schedule which contains information on the time-dependent values of the boundary condition.

Consider a simple example in which the water phase at nodes 5 and 6 of a mesh are subjected to prescribed water pressure head defined by schedule number 1 and side 3 of element 56 is subjected to a prescribed oil flux defined by schedule 2. Lines 17 and 18 of the main data file would then be given as

2	0	0	}	Line 17: NBC(I,1) for type-1 boundaries
0	1	0	}	Line 18: NSS(I,1) for type-2 boundaries

and lines 19 - 20 referencing the schedule numbers and node or element numbers would be given as

5	1	}	Line 19A: list of type-1 nodes and schedules for water phase	
6	1	}		
(omitted)			}	Line 19B: list of type-1 nodes and schedules for oil phase
(omitted)			}	Line 19C: list of type-1 nodes and schedules for gas phase
(omitted)			}	Line 20A: list of type-2 elements, sides and schedules for water
56	3	2	}	Line 20B: list of type-2 elements, sides and schedules for oil
(omitted)			}	Line 20C: list of type-2 elements, sides and schedules for gas

Note that since no type-1 nodes are indicated for the oil or gas phases and there are no type-2 elements for the water or gas phases, input lines for these are omitted.

4.2.4.2. Boundary conditions for transport. Boundary conditions for the transport model are referenced in a manner similar to that for flow, except for transport explicit input is given for type-1 (prescribed porous media concentration) or type-3 (prescribed flux). The default condition in the event that no explicit specification of a boundary condition is made is the type-2 condition - namely, zero normal concentration gradient which implies zero dispersive flux. For the type-1 condition, the boundary condition schedule will describe the time-dependent variation in concentration at a specified node. For the type-3 boundary condition, the code fixes the normal flux of a given species on a boundary segment according to one of two options selected. The type-3 "infiltration" condition takes the chemical flux equal to the product of a prescribed influent concentration in a phase times the normal phase velocity. The type-3 "boundary layer" condition takes the chemical flux equal to the diffusive flux through a boundary layer of prescribed thickness. For the infiltration condition, the schedule gives the time variation in the influent concentration of the specified phase. For the boundary layer condition, no schedule is necessary since the boundary layer flux is computed entirely within the program and requires no external specification. When employing type-3 infiltration boundary conditions, particular care should be given to ensure consistency in the specification of influent concentrations with the partition coefficients of the chemicals to maintain a physically meaningful system description as discussed in the section on boundary conditions in Chapter 3. Schedules for the transport problem are numbered independently of those for the flow problem. That is, if there are 20 flow schedules and 10 transport schedules, the numbering of the flow schedules will run from 1 to 10 and the transport schedules will go from 1 to 20. The user should therefore not confuse flow schedule 5, for example, with transport schedule 5.

4.2.4.3 Boundary condition schedules. A boundary condition schedule refers to a series of input lines describing piece-wise linear time variations in boundary conditions for either the flow or transport problem. Each schedule may be comprised of one or more subschedules which describes the linear variation in a boundary condition over a time interval. Each subschedule prescribes two real variables. The first variable on each line is the time of the subschedule and the second variable is the value of the boundary condition at this time. Linear interpolation of boundary conditions with time will be made. For example, a schedule with J subschedules will be of the form:

$$\begin{array}{ccc}
 J & T_1 & V_1 \\
 & T_2 & V_2 \\
 & T_3 & V_3 \\
 & \vdots & \vdots \\
 & T_j & V_j
 \end{array}$$

The schedules are used to prescribe values of the boundary conditions for a given problem. The V 's above may represent prescribed heads for type-1 flow boundary nodes, Darcy fluxes for type-2 flow boundary segments, porous media concentrations for type-1 transport nodes or influent

concentrations for type-3 infiltration boundary segments. The sign convention for fluid fluxes is negative for inward flux.

In prescribing boundary condition values, it is recommended to always "ramp" values over a small period of time rather than impose abrupt step-changes to avoid numerical oscillations that may lead to nonconvergence or deterioration of the mass balance accuracy. For example, if a problem involves a total simulation period of 80 days and it is desired to simulate an oil spill infiltrating under a pressure of $h_o = 0$ into an initially oil-free system, then the problem involves increasing the oil head from $h_o = h_o^{crit}$ to $h_o=0$ at $t=0$. Note that the value of h_o^{crit} may be easily obtained by checking the head in the output for $t=0$ when the program is run with IRUN=0. Say $h_o^{crit} = -0.67 \text{ m}$. To ramp the boundary conditions over a 0.1 day period the user can set up a schedule as follows:

3	0.0000	-0.670
	0.1000	0.00000
	10.000	0.00000

which increases the head over the 0.1 day period and then maintains a constant value. In creating boundary condition schedules, it is important to be sure to always have the final time in the schedule to equal or exceed the maximum simulation time *plus* the maximum time-step size to ensure that the boundary condition is defined over the entire period of the simulation.

5. PROGRAM APPLICATIONS

Three example problems will be discussed to demonstrate the use of MOFAT. Details of the simulations are described below. Information on computational effort required to perform the simulations on an 80386-based microcomputer are provided in Table 5.4.

5.1 Example 1. 1-D Spill of Two-Component Hydrocarbon

The first example problem involves a spill of a mixture of toluene and o-xylene at the soil surface followed by gradual leaching by rainfall. The domain of the problem is a 200 cm vertical section with a water table at a depth of 150 cm described by a single column of forty 5 x 5 cm elements using 82 nodes. Properties of the porous medium are given in Table 5.1. Note that since the problem is one dimensional, K_{sw_z} alone controls the flow. However, since the solution employs two dimensional elements K_{sw_z} is still employed. To minimize the possibility of oscillations in 1-D vertical problems, it is advisable to input $K_{sw_z} > K_{sw_x}$. Here, we use $K_{sw_z} = 2 K_{sw_x}$. The nonaqueous liquid entering the system is assumed to be composed of 50% mass fractions of toluene and o-xylene. The oil specific gravity, relative viscosity and scaling factors of the mixture estimated by [4.2] - [4.7] and the data in Table 4.2 are given in Table 5.1. Component values of air, oil and water phase diffusion coefficients, and oil-water and air-water partition coefficients estimated from [4.9] - [4.11] and the data in Table 4.2 are also summarized in Table 5.1. Solid-water partition coefficients and decay coefficients were assumed to be zero for both components. The problem is simulated in three stages involving one initial run and two restart runs as follows:

- Stage 1: Constant head oil infiltration
- Stage 2: Redistribution with transport for 25 days
- Stage 3: Constant flux water infiltration for 100 days

In Stage 1, oil infiltration is considered into soil which is initially oil-free and in equilibrium with a water table at a depth of 150 cm. Oil is added under a constant head of $h_o=0$ cm at the top two nodes under the JINF=2 option until the cumulative oil infiltration is $21 \text{ cm}^3 (=4.05 \text{ cm}^3 \text{cm}^{-2})$. Other boundaries for oil are no flow. The bottom nodes are maintained at a constant water head of $h_w=50$ cm corresponding to the initial conditions throughout Stage 1 and other boundaries are no flow for water. Transport is not considered during Stage 1 (ITRN=0) since the total duration of the first stage is only 0.0074 d. At the end of infiltration, the oil front is at a depth of approximately 20 cm (Figure 5.1).

Stage 2 involves a 25 day period during which oil redistribution occurs with no flow conditions at the upper boundary. Initial conditions for flow are read from the restart file. Transport is considered during Stage 2 with initial conditions computed internally using the KIC=1 option. Initial oil phase concentrations of toluene and o-xylene computed from [3.20] corresponding to 50% mass fractions are 436.7 mg cm^{-3} . Equilibrium water phase concentrations (CINIT) for toluene and xylene computed from [3.13a] are 0.2583 and $0.0762 \text{ mg cm}^{-3}$, respectively. Stage 2 is carried out for a period of 25 days with no flow boundary conditions for oil and with boundary

conditions for water as in Stage 1. Type-3 boundary conditions for transport are employed with the influent concentration, $C_{\alpha w}^{III}$, equal to zero corresponding to zero component mass flux on all boundaries. The water and total liquid saturation profiles at the end of Stage 2 are shown in Figure 5.1. Note that a residual oil saturation of about 7% occurs in the upper unsaturated zone due to a limitation on drainage under gravity when the oil permeability is low. Oil permeability increases near the water table as the water saturation increases resulting in faster oil drainage near the water table.

Table 5.1 Input parameters for Example 1.

<i>Soil properties:</i>		<i>Bulk fluid properties:</i>	
$K_{swz} = 800 \text{ cm d}^{-1}$		$\beta_{ao} = 2.1$	$\beta_{ow} = 1.83$
$K_{swz} = 400 \text{ cm d}^{-1}$		$\eta_{ro} = 0.695$	$\rho_{ro} = 0.873$
$\phi = 0.4$		<i>Component properties:</i>	
$S_m = 0.05$		o-Xylene	Toluene
$S_{or} = 0.2$		$D_{\alpha w}^o = 0.620$	$0.821 \text{ cm}^2 \text{ d}^{-1}$
$\alpha = 0.05 \text{ cm}^{-1}$		$D_{\alpha o}^o = 0.70$	$0.987 \text{ cm}^2 \text{ d}^{-1}$
$n = 2.5$		$D_{\alpha a}^o = 6099.$	$6765. \text{ cm}^2 \text{ d}^{-1}$
$A_L = 2.0 \text{ cm}$		$\Gamma_{\alpha o} = 5729.$	$1683.$
$A_T = 0.2 \text{ cm}$		$\Gamma_{\alpha a} = 0.22$	0.28
		$\rho_{\alpha} = 880.$	$862. \text{ mg cm}^{-3}$

Figure 5.1 Water and total liquid saturation vs depth at end of Stages 1, 2 and 3 for Example 1.

At the beginning of Stage 3, water infiltration is initiated at the upper surface at a constant flux of $q_w = 10 \text{ cm d}^{-1}$ via a type-2 flow boundary condition. The water head was maintained as in the previous stages at 50 cm at the bottom of the column. Zero oil flux was assumed on all boundaries. Initial conditions for flow and transport were read from a restart file from the end of Stage 2 (IRES=1 and KIC=1). Assuming infiltration of clean water, a type-3 transport boundary condition with $C_{\alpha w}^{III} = 0$ was imposed at the upper surface. At the lower surface and elsewhere a zero concentration gradient (type-2 condition) was employed to allow convective mass loss in the water phase from the bottom of the column.

Several different simulations of Stage 3 were run using both equilibrium and nonequilibrium interphase mass transfer analyses. To provide greater mass balance stability for the nonequilibrium analyses, the oil-based phase-summed transport formulation was employed. In

addition to an equilibrium simulation, analyses were performed using rate constants for all phase pairs of 1.0, 0.01 and 0.005 d^{-1} . Concentrations of xylene and toluene at the lower boundary are shown as a function of time for the various runs in Figure 5.2. Due to its higher solubility, toluene is lost from the system more rapidly than xylene leading to an increase in the mass fraction of xylene in the oil phase, and hence an increase in aqueous phase concentration at short times, followed by a reduction as extraction in the water phase continues. As the phase transfer rate constants increase to 1.0 d^{-1} , the nonequilibrium model is seen to give results identical to the equilibrium model. This degeneration to the equilibrium case provides verification of the nonequilibrium model formulation. As the rate coefficients decrease, the exit concentrations, and rate of leaching of contaminants from the oil phase, both diminish as expected.

Figure 5.2 Aqueous xylene and toluene concentrations at outflow boundary for Example 1 for equilibrium and nonequilibrium analyses. Rate coefficients in d^{-1} .

5.2 Example 2. 2-D Planar Spill with Sloping Water Table

This problem involves a light hydrocarbon spill in a two dimensional Cartesian section through saturated and unsaturated zones with a water table gradient. The problem is simulated in two stages involving one initial run and one restart run as follows:

Stage 1: Constant head oil infiltration on strip

Stage 2: Redistribution with transport for 25 days

The domain is 8 m in the vertical and 11 m in the horizontal with a water table initially located 4 m from the bottom on the left boundary and 3.5 m on the right. The lower surface is an aquitard and the top is the soil surface. An oil leak occurs on a strip 2 m in width centered 5 m from the left boundary along the top. Spatial discretization is achieved with 88 elements of 1 x 1 m spacing for a total of 108 nodes. Initially the water table is assumed to vary linearly from the left to right boundaries and water pressures are hydrostatic with no oil in the system. Boundary conditions for the water phase in Stage 1 are no flow on the top and bottom boundaries and prescribed head on the side corresponding to the initial conditions allowing water flow in the aquifer from the left to the right. Boundary conditions for oil are no flow except on the strip source. (Note: this presumes the physical domain is large enough that free oil never reaches the boundaries.) At the beginning of Stage 1, oil infiltration commences on the strip source under a constant head of $h_o = -0.1$ m and is continued until the total accumulation of oil is 1.0 m^3 (per m in the third dimension). The organic liquid is assumed to be 89.5% inert oil and 10.5% benzene. Soil properties and bulk fluid properties are given in Table 5.2. Transport is not simulated during Stage 1 which lasts for only 4.17 d .

During Stage 2 oil redistribution and benzene transport is simulated subject to the same boundary conditions for the water phase as in Stage 1 and with no flow for oil on all boundaries. A zero concentration gradient was imposed on the downstream boundary to allow mass loss with the

water phase by convection. The zero gradient condition was employed on the upper and lower surface which have zero fluid flux resulting in the equivalent of a zero mass flux condition for transport. On the upstream boundary, a type-3 condition with zero influent concentration was imposed. Stage 2 was continued for a period of 25 days during which time the solution indicated a mass loss of benzene due to dissolution and transport of about 2%. Contours of oil saturation and water and gas phase concentrations at the end of Stage 2 are shown in Figures 5.3 - 5.5.

Table 5.2 Input parameters for Example 2.

<i>Soil properties:</i>		<i>Bulk fluid properties:</i>	
$K_{s w_s} = 10.0 \text{ cm d}^{-1}$		$\beta_{ao} = 2.69$	$\beta_{ow} = 1.59$
$K_{s w_s} = 5.0 \text{ cm d}^{-1}$		$\eta_{ro} = 2.0$	$\rho_{ro} = 0.832$
$\phi = 0.35$		<i>Component properties (benzene)</i>	
$S_m = 0.05$		$D_{\alpha w}^o = 0.94 \times 10^{-4} \text{ m}^2 \text{d}^{-1}$	
$S_{or} = 0.2$		$D_{\alpha o}^o = 1.13 \times 10^{-4} \text{ m}^2 \text{d}^{-1}$	
$\alpha = 5.0 \text{ m}^{-1}$		$D_{\alpha a}^o = 0.763 \text{ m}^2 \text{d}^{-1}$	
$n = 2.8$		$\Gamma_{\alpha o} = 493.$	
$A_L = 0.2 \text{ m}$		$\Gamma_{\alpha a} = 0.24$	
$A_T = 0.04 \text{ m}$		$\rho_a = 0.87 \times 10^6 \text{ g m}^{-3}$	

Figure 5.3 Oil saturation contours at the end of Stage 2 for Example 2.

Figure 5.4 Water phase concentration contours (g m^{-3}) at the end of Stage 2 for Example 2.

Figure 5.5 Gas phase concentration contours (g m^{-3}) at the end of Stage 2 for Example 2.

5.3 Example 3. 2-D Radial Dense Solvent Spill with Vacuum Extraction

This problem involves a spill of tetrachloroethylene (PER) in a radial domain and remediation using vacuum extraction. The simulation is performed in three stages with two restarts as follows:

- Stage 1: Oil infiltration event
- Stage 2: Redistribution and transport under natural gradients
- Stage 3: Remediation using gas vacuum extraction

The first stage of the problem involves infiltration PER on a circular area with a radius of 2.0 *m* at the soil surface. A total of 3 *m*³ of NAPL is assumed to infiltrate under a water-equivalent oil head of -0.25 *m*. A water table occurs at a depth of 3.2 *m* and an impermeable layer occurs 5 *m* below the surface. The soil is uniform and has properties given in Table 5.3. Fluid properties for PER are also given in the table. The problem is analyzed as a 2-D radial section with an inner radius of 0.1 *m* (in order to facilitate subsequent analysis of pumping from a well of the same radius) and an outer radius of 8 *m*. A mesh with 12 nodes in the vertical direction and 16 nodes in the horizontal direction is employed.

Initial conditions for the water phase are assumed to correspond to equilibrium with the water table with no oil. Boundary conditions for the water phase involve a type-1 condition on the right side below the water table corresponding to vertical hydrostatic conditions (i.e., same as the initial conditions). All other boundaries are no flow for the water phase. Boundary conditions for the oil phase are a type-1 condition with $h_o = -0.25$ *m* on the 5 nodes on the upper surface between $r = 0$ and $r = 2.0$ *m*. All other nodes are no flow for oil. Gas flow was not considered during infiltration (NPH=2). Termination of Stage 1 occurred at $t = 6.48$ *d* after infiltration of 3.128 *m*³ of oil.

Stage 2 of the problem involves a continuation of the Stage 1 using the restart option (IRES=1). Redistribution of the PER is permitted for a period of 25 *d* under no flow boundary conditions for the oil phase on all boundaries. Boundary conditions for the water phase are maintained as in the infiltration stage. Gas phase flow is again disregarded. Transport is considered with the KIC=1 option and the initial aqueous concentration of PER at nodes with oil phase set to the solubility of 150 *g m*⁻³. Boundary conditions for transport are type-2 (zero dispersive flux) on all boundaries

which is equivalent to zero flux since there is essentially no flow on the boundaries during Stage 2. By the end of the redistribution period, the NAPL plume has reached the lower aquifer boundary. However, a substantial volume of the spill is still retained in the zone above the water table as "residual saturation" retained by capillary forces. The oil saturation distribution at the end of Stage 2 is shown in Figure 5.6.

In Stage 3, remediation is simulated with vacuum pumping in the unsaturated zone. A vacuum well with a 0.1 *m* radius is assumed to be placed at the left boundary screened over a 2.5 *m* interval from a depth of 1.25 *m* to 3.25 *m* and regulated at a pressure head of $h_a = -1.5$ *m*. The gas boundary at the well is treated as a type-1 boundary condition. Gas inflow is permitted along the upper surface from $r = 3.5$ *m* to the outer perimeter under a type-1 condition for gas with a constant pressure of $h_a = 0$. The inner 3.5 *m* of the surface, which is assumed covered, and other boundaries are treated as no flow for the gas phase. Water head is prescribed on the right boundary below the water table as in the earlier simulations and all other boundaries are treated as no flow for water. No flow conditions are imposed for the oil phase on all boundaries. Boundary conditions for transport are type-3 with zero influent concentration on the top and right side boundaries and zero dispersive flux elsewhere. Gas pumping results in water table upwelling as shown in Figure 5.7. The gas flow rate stabilizes at 319 *m*³ *d*⁻¹ after 2 days and the PER recovery rate reaches a corresponding steady rate of 16.77 *kg d*⁻¹. PER mass in the soil vs

venting time (Figure 5.8) shows a small increase (~ 1.5%) during the first day due to numerical error before the solution stabilizes and mass removal rate becomes nearly constant.

Table 5.3 Input parameters for Example 3.

<i>Soil properties:</i>	<i>Bulk fluid properties:</i>
$K_{s_{w_x}} = 5.0 \text{ cm } d^{-1}$	$\beta_{ao} = 2.3$ $\beta_{ow} = 1.77$
$K_{s_{w_x}} = 2.0 \text{ cm } d^{-1}$	$\eta_{ro} = 0.9$ $\rho_{ro} = 1.62$
$\phi = 0.4$	<i>Component properties (benzene)</i>
$S_m = 0.1$	$D_{\alpha_w}^o = 0.85 \times 10^{-4} \text{ m}^2 d^{-1}$
$S_{or} = 0.2$	$D_{\alpha_o}^o = 0.95 \times 10^{-4} \text{ m}^2 d^{-1}$
$\alpha = 3.0 \text{ m}^{-1}$	$D_{\alpha_a}^o = 0.65 \text{ m}^2 d^{-1}$
$n = 2.8$	$\Gamma_{\alpha_o} = 10,800.$
$A_L = 0.1 \text{ m}$	$\Gamma_{\alpha_a} = 0.35$
$A_T = 0.02 \text{ m}$	$\rho_{\alpha} = 1.62 \times 10^6 \text{ g m}^{-3}$

Figure 5.6 Oil saturation contours at the end of Stage 2 for Example 3.

Figure 5.7 Water saturation contours at the end of Stage 3 for Example 3.

Figure 5.8 PER mass in system vs time during Stage 3 of Example 3.

Table 5.4 Computaional effort required for example problems.

Problem	CPU time (min)*	Total number of time steps	Avg. iterations per time step
Example 1			
<i>Stage 1</i>	0.5	13	5.5
<i>Stage 2</i>	5.8	358	2.2
<i>Stage 3</i>	13.8	858	1.7
Example 2			
<i>Stage 1</i>	12.3	211	1.0
<i>Stage 2</i>	21.3	327	1.0
Example 3			
<i>Stage 1</i>	118.	203	3.5
<i>Stage 2</i>	139.	327	1.3
<i>Stage 3</i>	281.	260	3.0

* CPU time for 33 Mhz 80386 computer with Weitek 3167 coprocessor running under DOS compiled using NDP FORTRAN

6. REFERENCES

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APPENDIX A. DESCRIPTION OF MAIN INPUT FILE

1. Input Data for Flow Module

Line	Variable	Format	Description
1	TITLE	72A1	Description or title of the problem
2A	IRUN	I5	Index for execution control; = 0 reads and echoes input data = 1 executes the problem
	IRES	I5	Restart option: = 0 not a restart problem = 1 restart problem for number of phases same in previous and current problems = 2 restart problem for IAIR=0 in previous problem and IAIR=1 in current problem while IOIL=1 in both (see 4.2.3.1).
	IRAD	I5	Index to describe 2D flow problem: = 0 for plane section in x-z coordinates = 1 for radial section in r-z coordinates
	IOIL	I5	Index to describe if oil phase is active, = 0 oil phase equation not solved = 1 oil phase equation is solved (see 4.2.1.1)
	IAIR	I5	Index to describe if phase is active: = 0 gas phase equation not solved = 1 gas phase equation is solved(see 4.2.1.1)
	ITRN	I5	Index to include transport module: = 0 flow only = 1 flow and transport
	IDIM	I5	Index to specify the units of linear dimensions: = 1 for centimeters = 2 for meters (see 4.2.1.3)

IFEMC	I5	Index to activate ASD algorithm: = 0 ASD algorithm active = 1 ASD not active (see 2.2.4)
KFEMC	I5	Index to inactivate oil phase equation = 0 oil phase equation active = 1 oil equation inactive if $\Delta S_o < \text{TOL3}$ (see 4.2.1.8)

Note: Line 2B should be entered only if IFEMC = 0

2B	TOL1	E10.4	ASD tolerance for liquid phase pressures
	TOL2	E10.4	ASD tolerance for liquid phase saturations (see 2.2.4)

Note: Line 2C should be entered only if IFEMC=1 and KFEMC=1

2C	TOL3	E10.4	Tolerance for oil saturation for eq. elimination (see 4.2.1.8)
3	MXTST	I5	Maximum number of time steps allowed (see 4.2.1.5)
	MCNT	I5	Maximum number of iterations allowed
	NMAT	I5	Number of material types (max=10)
	ICN	I5	Number of flow boundary condition schedules (max=100)
	IROW	I5	Number of rows in the mesh
	KCOL	I5	Number of columns in the mesh
	KEQUL	I5	Index to describe interphase partition: = 0 local equilibrium between phases assumed = 1 nonequilibrium interphase mass partitioning
	IMCOR	I5	Index to activate mass injection scheme: = 0 mass injection scheme inactive = 1 mass injection scheme active (see Section 4.2.1.11)

ISOLVE	I5	Index to control matrix solution method: = 1 Solver A - more efficient but less robust = 2 Solver B - less efficient but more robust
ITPNT1	I5	Index for intermediate printout = 0 results are printed at all nodes = 1 results printed only at selected nodes

Note: The maximum number of nodes (IROW x KCOL) must not exceed 1500 and the maximum difference between node numbers of adjacent nodes must not exceed 50.

4A	ZCO(I) I=1,IROW	7E10.4	z-coordinates of the nodal points on the z-axis starting from the lower left corner [L]
4B	XCO(I) I=1,KCOL	7E10.4	X-coordinates of the nodal points on the x-axis starting from the lower left corner [L]
5	JINF	I5	Index for terminating the current run based on total change in phase volume in system: = 0 option inactive = 1 Water volume prescribed = 2 oil volume prescribed = 3 gas volume prescribed
	TINF	I5	Cumulative fluid intake (see 4.2.1.5) [L ³] program halts when phase accumulation>TINF (needed only if JINF >0)
6A	TIME	E10.4	Starting time of the simulation. Usually zero unless a restart problem [T]
	DELT	E10.4	Starting time increment [T]
	TMAX	E10.4	Maximum simulation time [T], (see 4.2.1.5)
	DTMX	E10.4	Maximum allowable time increment [T]
	TFACT	E10.4	Incremental factor for time-step (1.02-1.05)
	TPNT	E10.4	Time interval for printout of results [T]

Note: *Lines 6B and 6C should be entered only if ITPNT1= 1*

6B	ITPNT2	I5	Number of nodes where results are to be printed
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6C	ITPNT(I) I=1,ITPNT2	10I5	Nodes at which results are to be printed
7	VISOW	E10.4	Ratio of oil to water viscosity, η_{ro} [-]
	RHOW	E10.4	Ratio of oil to water phase density, ρ_{ro} [-] (not used if ITRN=1)
	BAO	E10.4	Air-oil phase scaling parameter, β_{ao} [-]
	BOW	E10.4	Oil-water phase scaling parameter, β_{ow} [-] (see 4.1.2)
8	TH	E10.4	Time weighting factor, $0.50 \leq \theta \leq 1.0$ $\theta=1$ refers to fully implicit scheme
	ABSA	E10.4	Absolute convergence limit for all fluid heads [L] (see 2.2.3)
	RCON	E10.4	Relative convergence limit for all phases [-] (see 2.2.3)
	UWF	E10.4	Upstream weighting coefficient for flow (see 2.2.1)

Note: Lines 9 to 11D are entered only if IRES=0

9	IUFW	I5	Index describing initial condition for water: = 0 water pressure from bilinear interpolation = 1 nonuniform water pressure distribution
	IUFO	I5	Index describing initial condition for oil = 0 oil pressure from bilinear interpolation = 1 no oil condition = 2 nonuniform oil pressure distribution

Note: Line 10A should be entered only if IUFW = 0

10A	WPI(1)	E10.4	Parameter a in eq. [4.16] for left boundary
	WPI(2)	E10.4	Parameter a in eq. [4.16] for right boundary

CWC	E10.4	Parameter b in equation [4.161]
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Note: Line 10B should be entered only if IUFO = 0

10B	OPI(1)	E10.4	Parameter c in eq. [4.17] for left boundary
	OPI(2)	E10.4	Parameter c in eq. [4.17] for right boundary
	COC	E10.4	Parameter d in equation [4.17]

Note: Line 11C should be entered only if IUFW = 1

11C	CHAF(I,1) I=1,NPT,NPH	7E10.4	Initial water heads entered sequentially for all nodes from node 1 to NXY=IROW x KCOL [L]
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Note: Line 11D should be entered only if IUFO=2

11D	CHAF(I,1) I=2,NP, NPH	7E10.4	Initial oil heads entered sequentially for all nodes from node 1 to NXY=IROWxKCOL [L]
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Note: Line 12 should be repeated NMAT times

12	PROP(5,I)	E10.4	K_{aw} in the x-direction for soil I [$L T^{-1}$]
	PROP(6,I)	E10.4	K_{sw} in the z-direction for soil I [$L T^{-1}$]
	PROP(4,I)	E10.4	Total porosity, ϕ , for soil I [-]
	PROP(2,I)	E10.4	Residual Water saturation, S_m , for soil I [-]
	PROP(8,I)	E10.4	Max. residual oil saturation, S_{or} , for soil I [-]
	PROP(1,I)	E10.4	Parameter α of VG model for soil I [L^{-1}]
	PROP(3,I)	E10.4	Parameter n of VG model, for soil I [-]

Note: Line 13 should be entered only if NMAT > 1

13	IMAT	I5	Index for assigning material types to nodes: = 1 material type read for blocks of nodes = 2 material types read for each node
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Note: Line 14 should be entered only if IMAT = 1

14A	KBL	I5	Number of blocks of nodes
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*Note: Line 14B should be read KBL times
(important: all nodes must be included in blocks!)*

14B	K1	I5	Lowest node number in block J
	K2	I5	Highest node number in block J
	K3	I5	Material type for block J

Note: Line 15 should be read only if IMAT = 2

15	IPROP(I) I=1,NXY	I5	Material type for node I (enter sequentially for all nodes from node 1 to NXY=IROWxKCOL)
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Note: Line 16 should be read only if IOIL=1 and IAIR=1

16	ICOM	I5	Index describing gas compressibility: = 0 compressible = 1 incompressible (see 4.2.1.9)
	TMXG	E10.4	Tolerance for deciding if gas flow is at steady-state. If changes in gas heads for all nodes in the domain are less than TMXG over a time-step, gas flow will be assumed steady and the gas equation will not be solved for subsequent time-steps (IAIR is set to 0). If ITRN=1, gas velocities in the transport equation will be fixed thereafter at the steady-state values. TMXG=0 forces continuous solution of gas flow equation. (see 4.2.1.9)

Note: Total numbers of type-1 and type-2 nodes for each phase must not exceed 100.

17	NBC(1,1)	I5	Total number of nodes with type-1 BC for water
	NBC(2,1)	I5	Total number of nodes with type-1 BC for oil
	NBC(3,1)	I5	Total number of nodes with type-1 BC for gas (see 4.2.4.1)

18	NSS(1,1)	I5	Total no. of elements with type-2 BC for water
	NSS(2,1)	I5	Total no. of elements with type-2 BC for oil
	NSS(3,1)	15	Total no. of elements with type-2 BC for gas (see 4.2.4.1)

Note: Line 19A is entered only if $NBC(1,1) > 0$ and is repeated $NBC(1,1)$ times

19A	NNB1(2,L,1)	I5	Number of the node with type-1 BC for water
	NNB1(1,L,1) L=1,NBC(1,1)	I5	Schedule number for this node

Note: Line 19B is entered only if $NBC(2,1) > 0$ and is repeated $NBC(2,1)$ times

19B	NNB2(2,L,1)	I5	Number of the node with type-1 BC for oil
	NNB2(1,L,1) L=1,NBC(2,1)	I5	Schedule number for this node

Note: Line 19C is entered only if $NBC(3,1) > 0$ and is repeated $NBC(3,1)$ times

19C	NNB3(2,L,1)	I5	Node number of the node with type-1 BC for gas
	NNB3(1,L,1) L=1,NBC(3,1)	I5	Schedule number for this node

Note: Line 20A is entered only if $NSS(1,1) > 0$ and is repeated $NSS(1,1)$ times

20A	NNSW(2,L,1)	I5	Number of element with type-2 BC for water
	NNSW(3,L,1)	I5	Side of the element exposed to flux BC
	NNSW(1,L,1) L=1,NSS(1,1)	I5	Schedule number for this element side

Note: Line 20B is entered only if $NSS(2,1) > 0$ and is repeated $NSS(2,1)$ times

20B	NNSO(2,L,1)	I5	Number of the element with type-2 BC for oil
	NNSO(3,L,1)	I5	Side of the element exposed to flux BC

NNSO(1,L,1)	I5	Schedule number for this element side
L=1,NSS(2,1)		

Note: Line 20C is entered only if NSS(3,1) > 0 and is repeated NSS(3,1) times

20C	NNSA(2,L,1)	I5	Number of the element with type-2 BC for gas
	NNSA(3,L,1)	I5	Side of the element exposed to flux BC
	NNSA(1,L,1)	I5	Schedule number for this element side
	L=1,NSS(3,1)		

Note: Lines 21 and 22 are repeated as a block ICN times to describe the ICN flow boundary condition schedules. For each schedule, line 21 should be given once and line 22 is repeated ISUB(L)-1 times. If there is only one subschedule for a given schedule (ISUB(L) = 1 then line 22 is omitted for that schedule.

21	ISUB(L)	I5	Number of subschedules in schedule L (max=4)
	CN(1,K,L)	E10.4	Time for subschedule K of schedule L
	CN(3,K,L)	E10.4	Value for subschedule K of schedule L
22	CN(1,K,L)	E10.4	Time for subschedule K of schedule L
	CN(3 K,L)	E10.4	Value for subschedule K of schedule L
	K=1,ISUB(L)		(see 4.2.4.3)
	L=1,ICN		

2. Input Data for Transport Module (enter if ITRN=1)

23	KUNIT	I5	Index to specify mass units: = 1 milligrams = 2 grams = 3 kilograms (see 4.2.1.3)
	NTSP	I5	Number of partitionable organic species to be simulated (max= 5)
	NCON(1)	I5	Total number of type-1 nodes for transport (max=100), (see 4:2.4-2)

	NEBC(1)	I5	Total number of type-3 elements for transport (max=100)
	KCN	I5	Total number of schedules describing transport boundary conditions (max=100)
	IEVAP	I5	Index to specify presence evaporative boundary = 0 evaporative boundary not present = 1 evaporative boundary is present
24	TRANS(1)	E10.4	Longitudinal dispersivity [L]
	TRANS(2)	E10.4	Transverse dispersivity, (see 3.1.1) [L]
	UWT	E10.4	Upstream weighting factor for transport [-]
	TTRN	E10.4	Time at which interphase mass transfer update starts, (see 4.2.1.10) [T]

Note: Line 25 should be repeated NTSP times

25	GAM(α ,1)	E10.4	Equilibrium partition coefficient between oil and water for species, (see 3.1.2) α [-]
	GAM(α ,2)	E10.4	Equilibrium partition coefficient between air and water for species α [-]
	GAM(α ,3)	E10.4	Equilibrium partition coefficient between solid and water for species of α [-]
	DCAY(α ,1)	E10.4	First order decay coefficient for species α in water phase, (see 3.1.1) [T ⁻¹]
	DCAY(α ,2)	E10.4	First order decay coefficient for species α in oil phase [T ⁻¹]
	DCAY(α ,3)	E10.4	First order decay coefficient for species α in air phase [T ⁻¹]
	DCAY(α ,4)	E10.4	First order decay coefficient for species α on solid phase [T ⁻¹]

Note: Line26A should be repeated NTSP times

26A	DIFW(α)	E10.4	Diffusion coefficient of species α in water [L^2T^{-1}] (see 3.1.1)
	DIFO(α)	E10.4	Diffusion coefficient of species α in oil [L^2T^{-1}]
	DIFA(α)	E10.4	Diffusion coefficient of species α in air [L^2T^{-1}]
	DLIQ(α)	E10.4	Liquid density of pure species α [$M L^{-3}$]

Note: Line 26B should be repeated NTSP times if KEQUL=1

26B	EPART($\alpha,1$)	E10.4	Water-gas mass transfer coefficient [T^{-1}] (see 3.1.3)
	EPART($\alpha,2$)	E10.4	Oil-water mass transfer coefficient [T^{-1}]
	EPART($\alpha,3$)	E10.4	Oil-gas mass transfer coefficient [T^{-1}]
	EPART($\alpha,4$)	E10.4	Water-solid mass transfer coefficient [T^{-1}]
	ABSC(α)	E10.4	Absolute convergence criteria for transport eqn in terms of water concentration [$M L^{-3}$] (see 4.2.1.6)
27	KIC	I5	Option for initial conditions for transport: = 0 assign zero concentration where $S_o = 0$ and specified constant values where $S_o \neq 0$ = 1 read initial concentrations from restart file = 2 read initial concentrations for all nodes from main data file (see 4.2.3.2)
	CINIT(K) K=1,NTSP	5E10.4	Initial water phase concentration for species K where $S_o \neq 0$ (needed if KIC=0 and IUFO \neq 1)

Note: Line 28 is entered only if KIC=2 and is repeated NTSP times.

28	CON(I, $\alpha,1$) I=1,NXY	7E10.4	Nonuniform initial water phase concentration of species α input serially for all nodes [$M L^{-3}$]
----	--------------------------------	--------	---

*Note: Line 29 should be entered only if $NCON(1) > 0$ and is repeated $NCON(1)$ time.
Omit $JSCH(J,1,\alpha)$ entries on each line for values of $\alpha > NTSP$.*

29	NSPB(J,1)	I5	Number of the node with type-1 BC
	JSCH(J,1,1)	I5	Schedule number for this node for species 1
	JSCH(J,1,2)	I5	Schedule number for this node for species 2
	JSCH(J,1,3)	I5	Schedule number for this node for species 3
	JSCH(J,1,4)	I5	Schedule number for this node for species 4
	JSCH(J,1,5)	I5	Schedule number for this node for species 5
	J=1,NCON(1)		(see 4.2.4.2)

*Note: Line 30 should be entered only if $NEBC(1) > 0$ and is repeated $NEBC(1)$ times.
Omit $KSCH(J,1,\alpha)$ entries on each line for values of $\alpha > NTSP$.*

30	IDBC(J,1,1)	I5	Number of element with type-3 BC (see 4.2.4.2)
	IDBC(J,1,2)	I5	Side number of the element with type-3 BC
	KSCH(J,1,1)	I5	Schedule number for species 1
	KSCH(J,1,2)	I5	Schedule number for species 2
	KSCH(J,1,3)	I5	Schedule number for species 3
	KSCH(J,1,4)	I5	Schedule number for species 4
	KSCH(J,1,5)	I5	Schedule number for species 5
	J=1,NEBC(1)		

Note: Lines 31 and 32 are repeated as a block KCN times to describe the KCN transport boundary condition schedules. For each schedule, line 31 should be given and line 32 is repeated $KSUB(L)-1$ times. If there is only one subschedule for a given schedule ($KSUB(L) = 1$) then line 32 will be omitted for that schedule (see 4.2.4.3).

31	KSUB(L)	I5	Number of subschedules in schedule L (max=4)
	ACN(1,K,L)	E10.4	Time for subschedule K of schedule L

	ACN(3,K,L)	E10.4	Value for subschedule K of schedule L
32	ACN(1,K,L)	E10.4	Time for subschedule K of schedule L
	ACN(3,K,L)	E10.4	Value for subschedule K of schedule L
	K=1,KSUB(L)		
	L=1,KCN		
		-----	END OF INPUT DATA

APPENDIX B. MAIN DATA FILES FOR EXAMPLE 2

EXAMPLE: 2A (INFILTRATION)

```

1 0 0 1 0 0 2 1 0
1000 30 1 10 9 12 0 0 2 0
0.0000 1.0000 2.0000 3.0000 4.0000 5.0000 6.0000
7.0000 8.0000
0.0000 1.0000 2.0000 3.0000 4.0000 5.0000 6.0000
7.0000 8.0000 9.0000 10.0000 11.0000
2 1.0000
0.0000 0.0005 100.0000 0.1500 1.0300 120.0000
2.0000 0.8320 2.6900 1.5900
1.0000 0.1000 0.0010 1.0000
0 1
4.0000 3.5000 -1.0000
10.0000 5.0000 0.3500 0.0500 0.2000 5.0000 2.8000
9 3 0
0 0 0
1 6
2 5
3 4
4 3
5 2
100 10
101 9
102 8
103 7
45 1
54 1
63 1
3 0.0000 -1.0000
0.005 -0.1000
9999.0000 -0.1000
2 0.0000 0.0000
9999.0000 0.0000
2 0.0000 1.0000
9999.0000 1.0000
2 0.0000 2.0000
9999.0000 2.0000
2 0.0000 3.0000
9999.0000 3.0000
2 0.0000 4.0000
9999.0000 4.0000
2 0.0000 0.5000
9999.0000 0.5000
2 0.0000 1.5000
9999.0000 1.5000
2 0.0000 2.5000
9999.0000 2.5000
2 0.0000 3.5000
9999.0000 3.5000
0 0 0 0 0 0
.00000000 .00000000 .00000000 .00000000 .00000000
0

```

EXAMPLE: 2B (REDISTRIBUTION)..

```

 1  1  0  1  0  1  2  1  0  0
1000 30  1 10  9 12  0  0  2  0
0.0000 1.0000 2.0000 3.0000 4.0000 5.0000 6.0000
7.0000 8.0000
0.0000 1.0000 2.0000 3.0000 4.0000 5.0000 6.0000
7.0000 8.0000 9.0000 10.0000 11.0000
0 0.0000
0.0000 0.0005 25.0000 0.1500 1.0300 120.0000
2.0000 0.8320 2.6900 1.5900
1.0000 0.1000 0.0010 1.0000
10.0000 5.0000 0.3500 0.0500 0.2000 5.0000 2.8000
9 3 0
0 0 0
1 6
2 5
3 4
4 3
5 2
100 10
101 9
102 8
103 7
45 1
54 1
63 1
3 0.0000 -0.1000 0.0001 -0.1000
0.0002 -0.1000
2 0.0000 0.0000
9999.0000 0.0000
2 0.0000 1.0000
9999.0000 1.0000
2 0.0000 2.0000
9999.0000 2.0000
2 0.0000 3.0000
9999.0000 3.0000
2 0.0000 4.0000
9999.0000 4.0000
2 0.0000 0.5000
9999.0000 0.5000
2 0.0000 1.5000
9999.0000 1.5000
2 0.0000 2.5000
9999.0000 2.5000
2 0.0000 3.5000
9999.0000 3.5000
2 2 0 8 1 0
0.20000000 0.0400000 1.0000000 2.00000
493.0000 0.2400000 .00000000 .00000000 .00000000 .00000000 .00000000
1000000.0 0.0020000 .00000000 .00000000 .00000000 .00000000 .00000000
.00009400 .00011320 0.7629000 877000.0
.00000010 .00000010 .00000100 827000.0
0 177.8910 0.7443000
1 4 1 0 0 0 0
2 4 1 0 0 0 0
3 4 1 0 0 0 0
4 4 1 0 0 0 0
5 4 1 0 0 0 0
6 4 1 0 0 0 0

```

7	4	1	0	0	0	0
8	4	1	0	0	0	0
2	.0000000	.0000000				
9999.00	.0000000					

APPENDIX C. MAIN OUPUT FILES FOR EXAMPLE 2 C1. OUTPUT FOR EXAMPLE 2A (STAGE 1 - INFILTRATION)

TITLE: EXAMPLE: 2A (INFILTRATION)

NUMBER OF NODES	=	108
NUMBER OF ELEMENTS	=	88
OIL PHASE INDEX, IOIL	=	1
GAS PHASE INDEX, IAIR	=	0
NUMBER OF ACTIVE PHASES	=	2
NUMBER OF ROWS	=	9
NUMBER OF COLUMNS	=	12

IRAD	=	0
IRES	=	0
IRUN	=	1
ITRN	=	0
IDIM	=	2
NO. OF SCHEDULES	=	10
IFEMC	=	1
KFEMC	=	0
ISOLVE	=	2

----TEMPORAL DATA ----

STARTING TIME	=	0.0000
TIME STEP AT T=0	=	0.0005
MAX. SIMULATION TIME	=	100.0000
MAX. TIME STEP	=	0.1500
T. INCREMENT FACTOR	=	1.0300
PRINT OUT T. INTERVAL	=	120.0000

----FLUID PROPERTIES DATA----

DENSITY RATIO (O/W)	=	0.8320
VISCOSITY RATIO (O/W)	=	2.0000
BAO	=	2.6900
BOW	=	1.5900

----CONTROL DATA-----

TIME WEIGHTING FACTOR	=	1.0000
ABSOLUTE CONVERGENCE	=	0.1000
RELATIVE ERROR	=	0.00100
UP. STREAM FACTOR FOR FLOW	=	1.00
MAX. CUM. INTAKE (TINF)	=	1.000
JINF	=	2
MAX. ITERATIONS	=	30
MAX. TIME STEPS	=	1000
TOL1	=	0.1000
TOL2	=	0.0002
TOL3	=	0.00020

ELEMENT NO -----NODES CONNECTED----

1	1	10	11	2
2	2	11	12	3
3	3	12	13	4
4	4	13	14	5
5	5	14	15	6
6	6	15	16	7
7	7	16	17	8
8	8	17	18	9
9	10	19	20	11
10	11	20	21	12
11	12	21	22	13
12	13	22	23	14
13	14	23	24	15
14	15	24	25	16
15	16	25	26	17
16	17	26	27	18

17	19	28	29	20
18	20	29	30	21
19	21	30	31	22
20	22	31	32	23
21	23	32	33	24
22	24	33	34	25
23	25	34	35	26
24	26	35	36	27
25	28	37	38	29
26	29	38	39	30
27	30	39	40	31
28	31	40	41	32
29	32	41	42	33
30	33	42	43	34
31	34	43	44	35
32	35	44	45	36
33	37	46	47	38
34	38	47	48	39
35	39	48	49	40
36	40	49	50	41
37	41	50	51	42
38	42	51	52	43
39	43	52	53	44
40	44	53	54	45
41	46	55	56	47
42	47	56	57	48
43	48	57	58	49
44	49	58	59	50
45	50	59	60	51
46	51	60	61	52
47	52	61	62	53
48	53	62	63	54
49	55	64	65	56
50	56	65	66	57
51	57	66	67	58
52	58	67	68	59
53	59	68	69	60
54	60	69	70	61
55	61	70	71	62
56	62	71	72	63
57	64	73	74	65
58	65	74	75	66
59	66	75	76	67
60	67	76	77	68
61	68	77	78	69
62	69	78	79	70
63	70	79	80	71
64	71	80	81	72
65	73	82	83	74
66	74	83	84	75
67	75	84	85	76
68	76	85	86	77
69	77	86	87	78
70	78	87	88	79
71	79	88	89	80
72	80	89	90	81
73	82	91	92	83
74	83	92	93	84
75	84	93	94	85
76	85	94	95	86
77	86	95	96	87
78	87	96	97	88
79	88	97	98	89
80	89	98	99	90
81	91	100	101	92
82	92	101	102	93
83	93	102	103	94
84	94	103	104	95
85	95	104	105	96
86	96	105	106	97
87	97	106	107	98
88	98	107	108	99

LINEAR INTERPOLATION COEFF FOR WATER

A1	A2	B
4.0000000	3.5000000	-1.0000000

-----MATERIAL PROPERTIES-----

--MATERIAL TYPE-- 1

KSWX	=	0.1000E+02
KRWY	=	0.5000E+01
POROSITY	=	0.3500
SM	=	0.0500
SROW	=	0.2000
ALPHA	=	5.0000
N	=	2.8000

NUMBER OF TYPE 1 BC NODES (W)	9
NUMBER OF TYPE 1 BC NODES (O)	3
NUMBER OF TYPE 1 BC NODES (G)	0
IXBC3	0

NUMBER OF TYPE 2 BC ELEMENTS (W)	0
NUMBER OF TYPE 2 BC ELEMENTS (O)	0
NUMBER OF TYPE 2 BC ELEMENTS (G)	0

NODE SCHEDULE(W)

1	6
2	5
3	4
4	3
5	2
100	10
101	9
102	8
103	7

NODE SCHEDULE(O)

45	1
54	1
63	1

BOUNDARY CONDITION SCHEDULES

0.0000	-1.0000	..SCHEDULE 1
0.0050	-0.1000	
9999.0000	-0.1000	
0.0000	0.0000	..SCHEDULE 2
9999.0000	0.0000	
0.0000	1.0000	..SCHEDULE 3
9999.0000	1.0000	
0.0000	2.0000	..SCHEDULE 4
9999.0000	2.0000	
0.0000	3.0000	..SCHEDULE 5
9999.0000	3.0000	
0.0000	4.0000	..SCHEDULE 6
9999.0000	4.0000	
0.0000	0.5000	..SCHEDULE 7
9999.0000	0.5000	
0.0000	1.5000	..SCHEDULE 8
9999.0000	1.5000	

```

0.0000    2.5000  ..SCHEDULE 9
9999.0000    2.5000

0.0000    3.5000  ..SCHEDULE 10
9999.0000    3.5000

**** END OF INPUT DATA ****

```

```

*****
NODE      PROP      X      Z
*****
 1         1      0.000000    0.000000
 2         1      0.000000    1.000000
 3         1      0.000000    2.000000
 4         1      0.000000    3.000000
 5         1      0.000000    4.000000
 6         1      0.000000    5.000000
 7         1      0.000000    6.000000
 8         1      0.000000    7.000000
 9         1      0.000000    8.000000
10         1      1.000000    0.000000
11         1      1.000000    1.000000
12         1      1.000000    2.000000
13         1      1.000000    3.000000
14         1      1.000000    4.000000
15         1      1.000000    5.000000
16         1      1.000000    6.000000
17         1      1.000000    7.000000
18         1      1.000000    8.000000
19         1      2.000000    0.000000
20         1      2.000000    1.000000
21         1      2.000000    2.000000
22         1      2.000000    3.000000
23         1      2.000000    4.000000
24         1      2.000000    5.000000
25         1      2.000000    6.000000
26         1      2.000000    7.000000
27         1      2.000000    8.000000
28         1      3.000000    0.000000
29         1      3.000000    1.000000
30         1      3.000000    2.000000
31         1      3.000000    3.000000
32         1      3.000000    4.000000
33         1      3.000000    5.000000
34         1      3.000000    6.000000
35         1      3.000000    7.000000
36         1      3.000000    8.000000
37         1      4.000000    0.000000
38         1      4.000000    1.000000
39         1      4.000000    2.000000
40         1      4.000000    3.000000
41         1      4.000000    4.000000
42         1      4.000000    5.000000
43         1      4.000000    6.000000
44         1      4.000000    7.000000
45         1      4.000000    8.000000
46         1      5.000000    0.000000
47         1      5.000000    1.000000
48         1      5.000000    2.000000
49         1      5.000000    3.000000
50         1      5.000000    4.000000
51         1      5.000000    5.000000
52         1      5.000000    6.000000
53         1      5.000000    7.000000
54         1      5.000000    8.000000
55         1      6.000000    0.000000
56         1      6.000000    1.000000
57         1      6.000000    2.000000
58         1      6.000000    3.000000
59         1      6.000000    4.000000
60         1      6.000000    5.000000
61         1      6.000000    6.000000
62         1      6.000000    7.000000
63         1      6.000000    8.000000
64         1      7.000000    0.000000
65         1      7.000000    1.000000
66         1      7.000000    2.000000

```

67	1	7.0000000	3.0000000
68	1	7.0000000	4.0000000
69	1	7.0000000	5.0000000
70	1	7.0000000	6.0000000
71	1	7.0000000	7.0000000
72	1	7.0000000	8.0000000
73	1	8.0000000	0.0000000
74	1	8.0000000	1.0000000
75	1	8.0000000	2.0000000
76	1	8.0000000	3.0000000
77	1	8.0000000	4.0000000
78	1	8.0000000	5.0000000
79	1	8.0000000	6.0000000
80	1	8.0000000	7.0000000
81	1	8.0000000	8.0000000
82	1	9.0000000	0.0000000
83	1	9.0000000	1.0000000
84	1	9.0000000	2.0000000
85	1	9.0000000	3.0000000
86	1	9.0000000	4.0000000
87	1	9.0000000	5.0000000
88	1	9.0000000	6.0000000
89	1	9.0000000	7.0000000
90	1	9.0000000	8.0000000
91	1	10.0000000	0.0000000
92	1	10.0000000	1.0000000
93	1	10.0000000	2.0000000
94	1	10.0000000	3.0000000
95	1	10.0000000	4.0000000
96	1	10.0000000	5.0000000
97	1	10.0000000	6.0000000
98	1	10.0000000	7.0000000
99	1	10.0000000	8.0000000
100	1	11.0000000	0.0000000
101	1	11.0000000	1.0000000
102	1	11.0000000	2.0000000
103	1	11.0000000	3.0000000
104	1	11.0000000	4.0000000
105	1	11.0000000	5.0000000
106	1	11.0000000	6.0000000
107	1	11.0000000	7.0000000
108	1	11.0000000	8.0000000

HALF BAND WIDTH= 22

NODE |----- HEADS ---| |----- SATURATIONS -----|

HW HO HA SW SO SA

.... INITIAL HEADS & SATURATIONS.....

1	4.0000	4.0000	0.0000	1.0000	0.0000	0.0000
2	3.0000	3.0000	0.0000	1.0000	0.0000	0.0000
3	2.0000	2.0000	0.0000	1.0000	0.0000	0.0000
4	1.0000	1.0000	0.0000	1.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
6	-1.0000	-0.3715	0.0000	0.1021	0.0000	0.8979
7	-2.0000	-0.7430	0.0000	0.0651	0.0000	0.9349
8	-3.0000	-1.1145	0.0000	0.0573	0.0000	0.9427
9	-4.0000	-1.4860	0.0000	0.0543	0.0000	0.9457
10	3.9545	3.9545	0.0000	1.0000	0.0000	0.0000
11	2.9545	2.9545	0.0000	1.0000	0.0000	0.0000
12	1.9545	1.9545	0.0000	1.0000	0.0000	0.0000
13	0.9545	0.9545	0.0000	1.0000	0.0000	0.0000
14	-0.0455	-0.0169	0.0000	0.9905	0.0000	0.0095
15	-1.0455	-0.3884	0.0000	0.0982	0.0000	0.9018
16	-2.0455	-0.7599	0.0000	0.0645	0.0000	0.9355
17	-3.0455	-1.1314	0.0000	0.0571	0.0000	0.9429
18	-4.0455	-1.5029	0.0000	0.0542	0.0000	0.9458
19	3.9091	3.9091	0.0000	1.0000	0.0000	0.0000
20	2.9091	2.9091	0.0000	1.0000	0.0000	0.0000
21	1.9091	1.9091	0.0000	1.0000	0.0000	0.0000
22	0.9091	0.9091	0.0000	1.0000	0.0000	0.0000
23	-0.0909	-0.0338	0.0000	0.9385	0.0000	0.0615
24	-1.0909	-0.4053	0.0000	0.0946	0.0000	0.9054

25	-2.0909	-0.7768	0.0000	0.0639	0.0000	0.9361
26	-3.0909	-1.1483	0.0000	0.0569	0.0000	0.9431
27	-4.0909	-1.5198	0.0000	0.0542	0.0000	0.9458
28	3.8636	3.8636	0.0000	1.0000	0.0000	0.0000
29	2.8636	2.8636	0.0000	1.0000	0.0000	0.0000
30	1.8636	1.8636	0.0000	1.0000	0.0000	0.0000
31	0.8636	0.8636	0.0000	1.0000	0.0000	0.0000
32	-0.1364	-0.0507	0.0000	0.8365	0.0000	0.1635
33	-1.1364	-0.4222	0.0000	0.0915	0.0000	0.9085
34	-2.1364	-0.7936	0.0000	0.0634	0.0000	0.9366
35	-3.1364	-1.1651	0.0000	0.0567	0.0000	0.9433
36	-4.1364	-1.5366	0.0000	0.0541	0.0000	0.9459
37	3.8182	3.8182	0.0000	1.0000	0.0000	0.0000
38	2.8182	2.8182	0.0000	1.0000	0.0000	0.0000
39	1.8182	1.8182	0.0000	1.0000	0.0000	0.0000
40	0.8182	0.8182	0.0000	1.0000	0.0000	0.0000
41	-0.1818	-0.0675	0.0000	0.7095	0.0000	0.2905
42	-1.1818	-0.4390	0.0000	0.0887	0.0000	0.9113
43	-2.1818	-0.8105	0.0000	0.0629	0.0000	0.9371
44	-3.1818	-1.1820	0.0000	0.0565	0.0000	0.9435
45	-4.1818	-1.5535	0.0000	0.0540	0.0000	0.9460
46	3.7727	3.7727	0.0000	1.0000	0.0000	0.0000
47	2.7727	2.7727	0.0000	1.0000	0.0000	0.0000
48	1.7727	1.7727	0.0000	1.0000	0.0000	0.0000
49	0.7727	0.7727	0.0000	1.0000	0.0000	0.0000
50	-0.2273	-0.0844	0.0000	0.5872	0.0000	0.4128
51	-1.2273	-0.4559	0.0000	0.0862	0.0000	0.9138
52	-2.2273	-0.8274	0.0000	0.0624	0.0000	0.9376
53	-3.2273	-1.1989	0.0000	0.0564	0.0000	0.9436
54	-4.2273	-1.5704	0.0000	0.0539	0.0000	0.9461
55	3.7273	3.7273	0.0000	1.0000	0.0000	0.0000
56	2.7273	2.7273	0.0000	1.0000	0.0000	0.0000
57	1.7273	1.7273	0.0000	1.0000	0.0000	0.0000
58	0.7273	0.7273	0.0000	1.0000	0.0000	0.0000
59	-0.2727	-0.1013	0.0000	0.4843	0.0000	0.5157
60	-1.2727	-0.4728	0.0000	0.0839	0.0000	0.9161
61	-2.2727	-0.8443	0.0000	0.0620	0.0000	0.9380
62	-3.2727	-1.2158	0.0000	0.0562	0.0000	0.9438
63	-4.2727	-1.5873	0.0000	0.0538	0.0000	0.9462
64	3.6818	3.6818	0.0000	1.0000	0.0000	0.0000
65	2.6818	2.6818	0.0000	1.0000	0.0000	0.0000
66	1.6818	1.6818	0.0000	1.0000	0.0000	0.0000
67	0.6818	0.6818	0.0000	1.0000	0.0000	0.0000
68	-0.3182	-0.1182	0.0000	0.4031	0.0000	0.5969
69	-1.3182	-0.4897	0.0000	0.0818	0.0000	0.9182
70	-2.3182	-0.8612	0.0000	0.0615	0.0000	0.9385
71	-3.3182	-1.2327	0.0000	0.0561	0.0000	0.9439
72	-4.3182	-1.6042	0.0000	0.0538	0.0000	0.9462
73	3.6364	3.6364	0.0000	1.0000	0.0000	0.0000
74	2.6364	2.6364	0.0000	1.0000	0.0000	0.0000
75	1.6364	1.6364	0.0000	1.0000	0.0000	0.0000
76	0.6364	0.6364	0.0000	1.0000	0.0000	0.0000
77	-0.3636	-0.1351	0.0000	0.3403	0.0000	0.6597
78	-1.3636	-0.5066	0.0000	0.0799	0.0000	0.9201
79	-2.3636	-0.8781	0.0000	0.0612	0.0000	0.9388
80	-3.3636	-1.2496	0.0000	0.0559	0.0000	0.9441
81	-4.3636	-1.6211	0.0000	0.0537	0.0000	0.9463
82	3.5909	3.5909	0.0000	1.0000	0.0000	0.0000
83	2.5909	2.5909	0.0000	1.0000	0.0000	0.0000
84	1.5909	1.5909	0.0000	1.0000	0.0000	0.0000
85	0.5909	0.5909	0.0000	1.0000	0.0000	0.0000
86	-0.4091	-0.1520	0.0000	0.2918	0.0000	0.7082
87	-1.4091	-0.5235	0.0000	0.0782	0.0000	0.9218
88	-2.4091	-0.8950	0.0000	0.0608	0.0000	0.9392
89	-3.4091	-1.2665	0.0000	0.0558	0.0000	0.9442
90	-4.4091	-1.6380	0.0000	0.0536	0.0000	0.9464
91	3.5455	3.5455	0.0000	1.0000	0.0000	0.0000
92	2.5455	2.5455	0.0000	1.0000	0.0000	0.0000
93	1.5455	1.5455	0.0000	1.0000	0.0000	0.0000
94	0.5455	0.5455	0.0000	1.0000	0.0000	0.0000
95	-0.4545	-0.1689	0.0000	0.2540	0.0000	0.7460
96	-1.4545	-0.5404	0.0000	0.0767	0.0000	0.9233
97	-2.4545	-0.9119	0.0000	0.0604	0.0000	0.9396
98	-3.4545	-1.2833	0.0000	0.0556	0.0000	0.9444
99	-4.4545	-1.6548	0.0000	0.0536	0.0000	0.9464
100	3.5000	3.5000	0.0000	1.0000	0.0000	0.0000
101	2.5000	2.5000	0.0000	1.0000	0.0000	0.0000
102	1.5000	1.5000	0.0000	1.0000	0.0000	0.0000
103	0.5000	0.5000	0.0000	1.0000	0.0000	0.0000
104	-0.5000	-0.1857	0.0000	0.2243	0.0000	0.7757
105	-1.5000	-0.5572	0.0000	0.0752	0.0000	0.9248

106	-2.5000	-0.9287	0.0000	0.0601	0.0000	0.9399
107	-3.5000	-1.3002	0.0000	0.0555	0.0000	0.9445
108	-4.5000	-1.6717	0.0000	0.0535	0.0000	0.9465

INITIAL VOLUME OF WATER = 16.6242
INITIAL VOLUME OF OIL = 0.0000

***** END OF INITIAL CONDITIONS *****

FINAL OUTPUT AT TIME= 7.688650

NODE -|- - - - -VELOCITIES- - - - - -|-

	QW-X	QW-Y	QO-X	QO-Y	QA-X	QA-Y
1	0.4221E+00	0.0000E+00	0.1017E-06	0.2706E-06	0.0000E+00	0.0000E+00
2	0.4185E+00	0.0000E+00	0.9894E-07	0.2706E-06	0.0000E+00	0.0000E+00
3	0.4062E+00	0.0000E+00	0.9633E-07	0.3962E-06	0.0000E+00	0.0000E+00
4	0.3802E+00	0.0000E+00	0.8595E-07	0.4016E-06	0.0000E+00	0.0000E+00
5	0.3470E+00	0.0000E+00	0.7822E-07	0.3545E-06	0.0000E+00	0.0000E+00
6	-0.7999E-06	0.1597E+01	-0.6475E-07	-0.8472E-06	0.0000E+00	0.0000E+00
7	0.4426E-06	-0.1584E-05	0.8164E-07	-0.1445E-05	0.0000E+00	0.0000E+00
8	0.4014E-06	-0.3245E-08	0.7232E-07	-0.1152E-05	0.0000E+00	0.0000E+00
9	0.3052E-06	0.6060E-07	0.4740E-07	-0.1124E-05	0.0000E+00	0.0000E+00
10	0.4221E+00	-0.1785E-02	0.1017E-06	0.2692E-06	0.0000E+00	0.0000E+00
11	0.4185E+00	-0.1785E-02	0.9894E-07	0.2692E-06	0.0000E+00	0.0000E+00
12	0.4062E+00	-0.6135E-02	0.9633E-07	0.3949E-06	0.0000E+00	0.0000E+00
13	0.3802E+00	-0.1299E-01	0.8595E-07	0.3964E-06	0.0000E+00	0.0000E+00
14	0.3470E+00	-0.1481E-01	0.7822E-07	0.3506E-06	0.0000E+00	0.0000E+00
15	-0.7999E-06	0.1141E+01	-0.6475E-07	-0.9187E-06	0.0000E+00	0.0000E+00
16	0.4426E-06	-0.1189E-05	0.8164E-07	-0.1372E-05	0.0000E+00	0.0000E+00
17	0.4014E-06	-0.2385E-07	0.7232E-07	-0.1156E-05	0.0000E+00	0.0000E+00
18	0.3052E-06	0.1250E-07	0.4740E-07	-0.1137E-05	0.0000E+00	0.0000E+00
19	0.4253E+00	-0.3245E-02	0.1930E-06	0.2681E-06	0.0000E+00	0.0000E+00
20	0.4224E+00	-0.3245E-02	0.1908E-06	0.2681E-06	0.0000E+00	0.0000E+00
21	0.4126E+00	-0.1103E-01	0.1870E-06	0.3930E-06	0.0000E+00	0.0000E+00
22	0.3910E+00	-0.2378E-01	0.1772E-06	0.3915E-06	0.0000E+00	0.0000E+00
23	0.3143E+00	-0.2828E-01	0.6410E-07	0.2941E-06	0.0000E+00	0.0000E+00
24	-0.9549E-06	0.6517E+00	-0.6489E-07	-0.9832E-06	0.0000E+00	0.0000E+00
25	-0.1116E-06	-0.1070E-05	-0.1900E-06	-0.1435E-05	0.0000E+00	0.0000E+00
26	-0.2646E-05	-0.1291E-05	-0.1425E-05	-0.1774E-05	0.0000E+00	0.0000E+00
27	-0.4347E-05	-0.8379E-06	-0.2217E-05	-0.1533E-05	0.0000E+00	0.0000E+00
28	0.4313E+00	-0.4166E-02	0.2167E-06	0.2676E-06	0.0000E+00	0.0000E+00
29	0.4294E+00	-0.4166E-02	0.2158E-06	0.2676E-06	0.0000E+00	0.0000E+00
30	0.4237E+00	-0.1388E-01	0.2129E-06	0.3915E-06	0.0000E+00	0.0000E+00
31	0.4127E+00	-0.2922E-01	0.2060E-06	0.3881E-06	0.0000E+00	0.0000E+00
32	0.2534E+00	-0.3416E-01	0.6540E-07	0.2238E-06	0.0000E+00	0.0000E+00
33	-0.1166E-05	0.2691E+00	-0.8122E-07	-0.1056E-05	0.0000E+00	0.0000E+00
34	-0.3291E-05	-0.2535E-05	-0.1632E-04	-0.2086E-04	0.0000E+00	0.0000E+00
35	-0.6014E-05	-0.2653E-05	-0.2419E-02	-0.1860E-02	0.0000E+00	0.0000E+00
36	-0.6509E-05	-0.1086E-05	-0.1109E-03	-0.5249E-04	0.0000E+00	0.0000E+00
37	0.4390E+00	-0.4508E-02	0.2227E-06	0.2675E-06	0.0000E+00	0.0000E+00
38	0.4383E+00	-0.4508E-02	0.2224E-06	0.2675E-06	0.0000E+00	0.0000E+00
39	0.4370E+00	-0.1455E-01	0.2214E-06	0.3910E-06	0.0000E+00	0.0000E+00
40	0.4386E+00	-0.2831E-01	0.2168E-06	0.3858E-06	0.0000E+00	0.0000E+00
41	0.1798E+00	-0.3042E-01	0.6815E-07	0.1495E-06	0.0000E+00	0.0000E+00
42	-0.1297E-05	0.5011E-01	-0.1684E-06	-0.1175E-05	0.0000E+00	0.0000E+00
43	-0.1506E-05	-0.3096E-05	-0.7888E-03	-0.2344E-02	0.0000E+00	0.0000E+00
44	-0.5634E-06	-0.2181E-05	-0.5834E-02	-0.3393E-01	0.0000E+00	0.0000E+00
45	0.1064E-05	-0.2721E-06	-0.3191E-01	-0.6187E-01	0.0000E+00	0.0000E+00
46	0.4476E+00	-0.4401E-02	0.2254E-06	0.2675E-06	0.0000E+00	0.0000E+00
47	0.4478E+00	-0.4401E-02	0.2255E-06	0.2675E-06	0.0000E+00	0.0000E+00
48	0.4496E+00	-0.1363E-01	0.2256E-06	0.3911E-06	0.0000E+00	0.0000E+00
49	0.4588E+00	-0.2354E-01	0.2292E-06	0.3876E-06	0.0000E+00	0.0000E+00
50	0.1112E+00	-0.2122E-01	0.7171E-07	0.7071E-07	0.0000E+00	0.0000E+00
51	-0.1275E-05	-0.7014E-06	-0.2007E-06	-0.1311E-05	0.0000E+00	0.0000E+00
52	-0.1645E-06	-0.2988E-05	-0.1080E-02	-0.1273E-01	0.0000E+00	0.0000E+00
53	0.1547E-06	-0.2022E-05	-0.1816E-02	-0.6047E-01	0.0000E+00	0.0000E+00
54	0.2737E-06	-0.2126E-06	0.0000E+00	-0.6092E-01	0.0000E+00	0.0000E+00
55	0.4561E+00	-0.4047E-02	0.2277E-06	0.2676E-06	0.0000E+00	0.0000E+00
56	0.4568E+00	-0.4047E-02	0.2278E-06	0.2676E-06	0.0000E+00	0.0000E+00
57	0.4599E+00	-0.1210E-01	0.2290E-06	0.3916E-06	0.0000E+00	0.0000E+00
58	0.4689E+00	-0.1883E-01	0.2341E-06	0.3902E-06	0.0000E+00	0.0000E+00

59	0.5852E-01	-0.1320E-01	0.7283E-07	-0.9907E-08	0.0000E+00	0.0000E+00
60	-0.1146E-05	-0.2572E-05	0.1106E-06	-0.1292E-05	0.0000E+00	0.0000E+00
61	0.7716E-06	-0.2486E-05	0.1172E-02	-0.2035E-02	0.0000E+00	0.0000E+00
62	0.4305E-06	-0.2192E-05	0.1905E-02	-0.3309E-01	0.0000E+00	0.0000E+00
63	0.3197E-06	-0.2681E-06	0.0000E+00	-0.6193E-01	0.0000E+00	0.0000E+00
64	0.4642E+00	-0.3625E-02	0.2297E-06	0.2677E-06	0.0000E+00	0.0000E+00
65	0.4650E+00	-0.3625E-02	0.2299E-06	0.2677E-06	0.0000E+00	0.0000E+00
66	0.4678E+00	-0.1073E-01	0.2311E-06	0.3922E-06	0.0000E+00	0.0000E+00
67	0.4719E+00	-0.1652E-01	0.2357E-06	0.3925E-06	0.0000E+00	0.0000E+00
68	0.2650E-01	-0.8860E-02	0.6741E-07	-0.9406E-07	0.0000E+00	0.0000E+00
69	0.2622E-06	-0.3694E-05	0.8794E-07	-0.1282E-05	0.0000E+00	0.0000E+00
70	0.2115E-05	-0.1455E-05	0.7176E-03	-0.1812E-04	0.0000E+00	0.0000E+00
71	0.1164E-05	-0.2668E-05	0.5653E-02	-0.1857E-02	0.0000E+00	0.0000E+00
72	-0.4242E-06	-0.1062E-05	0.3206E-01	-0.5166E-04	0.0000E+00	0.0000E+00
73	0.4713E+00	-0.3133E-02	0.2313E-06	0.2679E-06	0.0000E+00	0.0000E+00
74	0.4723E+00	-0.3133E-02	0.2316E-06	0.2679E-06	0.0000E+00	0.0000E+00
75	0.4743E+00	-0.9715E-02	0.2329E-06	0.3929E-06	0.0000E+00	0.0000E+00
76	0.4745E+00	-0.1617E-01	0.2367E-06	0.3944E-06	0.0000E+00	0.0000E+00
77	0.1044E-01	-0.7672E-02	0.5157E-07	-0.1866E-06	0.0000E+00	0.0000E+00
78	0.2448E-05	-0.2563E-05	0.9286E-07	-0.1261E-05	0.0000E+00	0.0000E+00
79	0.4510E-05	0.2496E-05	0.1763E-04	-0.1167E-05	0.0000E+00	0.0000E+00
80	0.6778E-05	-0.1534E-05	0.2490E-02	-0.1897E-05	0.0000E+00	0.0000E+00
81	0.7165E-05	0.8685E-06	0.1123E-03	-0.1543E-05	0.0000E+00	0.0000E+00
82	0.4773E+00	-0.2337E-02	0.2308E-06	0.2683E-06	0.0000E+00	0.0000E+00
83	0.4789E+00	-0.2337E-02	0.2316E-06	0.2683E-06	0.0000E+00	0.0000E+00
84	0.4816E+00	-0.8368E-02	0.2343E-06	0.3942E-06	0.0000E+00	0.0000E+00
85	0.4793E+00	-0.1701E-01	0.2392E-06	0.3969E-06	0.0000E+00	0.0000E+00
86	0.3362E-02	-0.8915E-02	0.2720E-07	-0.2926E-06	0.0000E+00	0.0000E+00
87	0.3453E-05	-0.7527E-06	0.1480E-06	-0.1201E-05	0.0000E+00	0.0000E+00
88	0.1273E-05	0.2302E-05	0.4821E-06	-0.1000E-05	0.0000E+00	0.0000E+00
89	0.4311E-05	-0.1503E-07	0.1966E-05	-0.1155E-05	0.0000E+00	0.0000E+00
90	0.6060E-05	0.5821E-08	0.2781E-05	-0.1136E-05	0.0000E+00	0.0000E+00
91	0.4818E+00	-0.1336E-02	0.2160E-06	0.2715E-06	0.0000E+00	0.0000E+00
92	0.4838E+00	-0.1336E-02	0.2224E-06	0.2715E-06	0.0000E+00	0.0000E+00
93	0.4915E+00	-0.4511E-02	0.2347E-06	0.4003E-06	0.0000E+00	0.0000E+00
94	0.4892E+00	-0.1782E-01	0.2446E-06	0.4018E-06	0.0000E+00	0.0000E+00
95	-0.4673E-03	-0.1411E-01	-0.4665E-08	-0.4172E-06	0.0000E+00	0.0000E+00
96	0.2195E-05	0.2502E-02	0.1442E-06	-0.1126E-05	0.0000E+00	0.0000E+00
97	0.4639E-06	0.1256E-05	0.8648E-07	-0.1029E-05	0.0000E+00	0.0000E+00
98	0.5026E-06	0.4344E-08	0.9557E-07	-0.1150E-05	0.0000E+00	0.0000E+00
99	0.6111E-06	0.6004E-07	0.1274E-06	-0.1120E-05	0.0000E+00	0.0000E+00
100	0.4841E+00	0.0000E+00	0.1000E-06	0.3178E-06	0.0000E+00	0.0000E+00
101	0.4868E+00	0.0000E+00	0.1926E-06	0.3178E-06	0.0000E+00	0.0000E+00
102	0.4958E+00	0.0000E+00	0.2306E-06	0.4193E-06	0.0000E+00	0.0000E+00
103	0.5307E+00	0.0000E+00	0.2632E-06	0.4181E-06	0.0000E+00	0.0000E+00
104	-0.9411E-02	-0.3698E-01	-0.5547E-07	-0.5765E-06	0.0000E+00	0.0000E+00
105	0.8317E-06	0.1581E-01	0.8086E-07	-0.1058E-05	0.0000E+00	0.0000E+00
106	0.4422E-06	0.1020E-05	0.8188E-07	-0.1029E-05	0.0000E+00	0.0000E+00
107	0.4196E-06	-0.6946E-08	0.7725E-07	-0.1153E-05	0.0000E+00	0.0000E+00
108	0.3872E-06	0.4384E-07	0.7031E-07	-0.1123E-05	0.0000E+00	0.0000E+00

NODE |----- HEADS ---| |----- SATURATIONS ----|

	HW	HO	HA	SW	SO	SA
1	4.0000	3.8999	0.0000	1.0000	0.0000	0.0000
2	3.0000	2.9597	0.0000	1.0000	0.0000	0.0000
3	2.0000	1.9692	0.0000	1.0000	0.0000	0.0000
4	1.0000	0.9765	0.0000	1.0000	0.0000	0.0000
5	0.0000	0.0027	0.0000	1.0000	0.0000	0.0000
6	-1.3201	-0.4904	0.0000	0.0817	0.0000	0.9183
7	-2.0033	-0.7443	0.0000	0.0650	0.0000	0.9350
8	-3.0026	-1.1157	0.0000	0.0573	0.0000	0.9427
9	-4.0147	-1.4979	0.0000	0.0543	0.0000	0.9457
10	3.9578	3.8796	0.0000	1.0000	0.0000	0.0000
11	2.9582	2.9399	0.0000	1.0000	0.0000	0.0000
12	1.9594	1.9499	0.0000	1.0000	0.0000	0.0000
13	0.9620	0.9593	0.0000	1.0000	0.0000	0.0000
14	-0.0348	-0.0129	0.0000	0.9952	0.0003	0.0045
15	-1.2852	-0.4774	0.0000	0.0833	0.0000	0.9167
16	-2.0475	-0.7607	0.0000	0.0644	0.0000	0.9356
17	-3.0427	-1.1301	0.0000	0.0571	0.0000	0.9429
18	-4.0452	-1.5074	0.0000	0.0543	0.0000	0.9457
19	3.9153	3.8410	0.0000	1.0000	0.0000	0.0000
20	2.9159	2.9017	0.0000	1.0000	0.0000	0.0000
21	1.9181	1.9125	0.0000	1.0000	0.0000	0.0000
22	0.9229	0.9239	0.0000	1.0000	0.0000	0.0000
23	-0.0693	-0.0257	0.0000	0.9696	0.0004	0.0300

24	-1.2503	-0.4645	0.0000	0.0850	0.0000	0.9150
25	-2.0364	-0.7227	0.0000	0.0639	0.0019	0.9342
26	-2.7781	-0.8451	0.0000	0.0569	0.0050	0.9381
27	-3.6106	-1.0640	0.0000	0.0542	0.0037	0.9421
28	3.8721	3.7976	0.0000	1.0000	0.0000	0.0000
29	2.8730	2.8586	0.0000	1.0000	0.0000	0.0000
30	1.8757	1.8699	0.0000	1.0000	0.0000	0.0000
31	0.8816	0.8827	0.0000	1.0000	0.0000	0.0000
32	-0.1045	-0.0388	0.0000	0.9121	0.0005	0.0874
33	-1.2143	-0.4482	0.0000	0.0866	0.0007	0.9127
34	-1.7073	-0.3644	0.0000	0.0634	0.0406	0.8961
35	-2.1767	-0.1919	0.0000	0.0566	0.1584	0.7850
36	-2.9596	-0.3182	0.0000	0.0540	0.0646	0.8814
37	3.8282	3.7531	0.0000	1.0000	0.0000	0.0000
38	2.8291	2.8141	0.0000	1.0000	0.0000	0.0000
39	1.8320	1.8257	0.0000	1.0000	0.0000	0.0000
40	0.8377	0.8393	0.0000	1.0000	0.0000	0.0000
41	-0.1412	-0.0524	0.0000	0.8233	0.0004	0.1763
42	-1.1760	-0.4145	0.0000	0.0870	0.0059	0.9071
43	-1.5567	-0.1859	0.0000	0.0629	0.1611	0.7760
44	-2.1204	-0.1142	0.0000	0.0565	0.3639	0.5796
45	-3.0660	-0.1000	0.0000	0.0532	0.4383	0.5085
46	3.7835	3.7080	0.0000	1.0000	0.0000	0.0000
47	2.7844	2.7690	0.0000	1.0000	0.0000	0.0000
48	1.7871	1.7806	0.0000	1.0000	0.0000	0.0000
49	0.7918	0.7935	0.0000	1.0000	0.0000	0.0000
50	-0.1798	-0.0668	0.0000	0.7149	0.0004	0.2847
51	-1.1379	-0.3744	0.0000	0.0868	0.0146	0.8986
52	-1.5402	-0.1407	0.0000	0.0624	0.2604	0.6772
53	-2.1359	-0.1011	0.0000	0.0563	0.4290	0.5147
54	-3.0933	-0.1000	0.0000	0.0532	0.4384	0.5085
55	3.7379	3.6625	0.0000	1.0000	0.0000	0.0000
56	2.7387	2.7234	0.0000	1.0000	0.0000	0.0000
57	1.7411	1.7348	0.0000	1.0000	0.0000	0.0000
58	0.7449	0.7467	0.0000	1.0000	0.0000	0.0000
59	-0.2190	-0.0813	0.0000	0.6078	0.0005	0.3917
60	-1.1146	-0.3965	0.0000	0.0911	0.0053	0.9036
61	-1.6174	-0.1897	0.0000	0.0620	0.1562	0.7818
62	-2.1789	-0.1149	0.0000	0.0562	0.3614	0.5825
63	-3.1253	-0.1000	0.0000	0.0531	0.4384	0.5085
64	3.6915	3.6165	0.0000	1.0000	0.0000	0.0000
65	2.6922	2.6774	0.0000	1.0000	0.0000	0.0000
66	1.6943	1.6885	0.0000	1.0000	0.0000	0.0000
67	0.6976	0.6995	0.0000	1.0000	0.0000	0.0000
68	-0.2553	-0.0948	0.0000	0.5208	0.0004	0.4788
69	-1.1199	-0.4141	0.0000	0.0923	0.0006	0.9071
70	-1.8289	-0.3729	0.0000	0.0616	0.0402	0.8982
71	-2.2953	-0.1923	0.0000	0.0560	0.1584	0.7856
72	-3.0829	-0.3192	0.0000	0.0537	0.0646	0.8818
73	3.6443	3.5703	0.0000	1.0000	0.0000	0.0000
74	2.6449	2.6311	0.0000	1.0000	0.0000	0.0000
75	1.6469	1.6420	0.0000	1.0000	0.0000	0.0000
76	0.6501	0.6522	0.0000	1.0000	0.0000	0.0000
77	-0.2830	-0.1051	0.0000	0.4638	0.0003	0.5359
78	-1.1648	-0.4327	0.0000	0.0897	0.0000	0.9103
79	-2.2799	-0.7978	0.0000	0.0612	0.0021	0.9367
80	-2.9731	-0.8711	0.0000	0.0560	0.0053	0.9387
81	-3.7994	-1.0857	0.0000	0.0538	0.0038	0.9424
82	3.5966	3.5241	0.0000	1.0000	0.0000	0.0000
83	2.5971	2.5848	0.0000	1.0000	0.0000	0.0000
84	1.5987	1.5951	0.0000	1.0000	0.0000	0.0000
85	0.6021	0.6044	0.0000	1.0000	0.0000	0.0000
86	-0.2977	-0.1106	0.0000	0.4369	0.0003	0.5628
87	-1.2444	-0.4623	0.0000	0.0853	0.0000	0.9147
88	-2.4073	-0.8942	0.0000	0.0608	0.0000	0.9392
89	-3.4043	-1.2642	0.0000	0.0558	0.0000	0.9442
90	-4.4054	-1.6419	0.0000	0.0537	0.0000	0.9463
91	3.5484	3.4809	0.0000	1.0000	0.0000	0.0000
92	2.5487	2.5403	0.0000	1.0000	0.0000	0.0000
93	1.5496	1.5482	0.0000	1.0000	0.0000	0.0000
94	0.5531	0.5555	0.0000	1.0000	0.0000	0.0000
95	-0.2952	-0.1097	0.0000	0.4414	0.0003	0.5583
96	-1.3221	-0.4911	0.0000	0.0816	0.0000	0.9183
97	-2.4537	-0.9115	0.0000	0.0604	0.0000	0.9396
98	-3.4545	-1.2834	0.0000	0.0556	0.0000	0.9444
99	-4.4665	-1.6674	0.0000	0.0536	0.0000	0.9464
100	3.5000	3.4609	0.0000	1.0000	0.0000	0.0000
101	2.5000	2.5018	0.0000	1.0000	0.0000	0.0000
102	1.5000	1.5021	0.0000	1.0000	0.0000	0.0000
103	0.5000	0.5028	0.0000	1.0000	0.0000	0.0000
104	-0.2653	-0.0986	0.0000	0.4994	0.0002	0.5004

105	-1.3656	-0.5073	0.0000	0.0798	0.0001	0.9201
106	-2.4979	-0.9279	0.0000	0.0601	0.0000	0.9399
107	-3.4965	-1.2988	0.0000	0.0555	0.0000	0.9445
108	-4.5053	-1.6815	0.0000	0.0535	0.0000	0.9465

FINAL VOLUME OF WATER =	17.0398
FINAL VOLUME OF OIL =	1.0153

TOTAL ITERATIONS	217
TOTAL TIME STEPS	211

OUTPUT FOR EXAMPLE 2B (STAGE 1 - REDISTRIBUTION)

TITLE: EXAMPLE: 2B (REDISTRIBUTION)..

NUMBER OF NODES	=	108
NUMBER OF ELEMENTS	=	88
OIL PHASE INDEX, IOIL	=	1
GAS PHASE INDEX, IAIR	=	0
NUMBER OF ACTIVE PHASES	=	2
NUMBER OF ROWS	=	9
NUMBER OF COLUMNS	=	12

IRAD	=	0
IRES	=	1
IRUN	=	1
ITRN	=	1
IDIM	=	2
NO. OF SCHEDULES	=	10
IFEMC	=	1
KFEMC	=	0
ISOLVE	=	2

----TEMPORAL DATA -----

STARTING TIME	=	0.0000
TIME STEP AT T=0	=	0.0005
MAX. SIMULATION TIME	=	25.0000
MAX. TIME STEP	=	0.1500
T. INCREMENT FACTOR	=	1.0300
PRINT OUT T. INTERVAL	=	120.0000

----FLUID PROPERTIES DATA----

DENSITY RATIO (O/W)	=	0.8320
VISCOSITY RATIO (O/W)	=	2.0000
BAO	=	2.6900
BOW	=	1.5900

----CONTROL DATA-----

TIME WEIGHTING FACTOR	=	1.0000
ABSOLUTE CONVERGENCE	=	0.1000
RELATIVE ERROR	=	0.00100
UP. STREAM FACTOR FOR FLOW	=	1.00
MAX. CUM. INTAKE (TINF)	=	0.000
JINF	=	0
MAX. ITERATIONS	=	30
MAX. TIME STEPS	=	1000
TOL1	=	0.1000
TOL2	=	0.0002
TOL3	=	0.00020

ELEMENT NO -----NODES CONNECTED----

1	1	10	11	2
2	2	11	12	3
3	3	12	13	4
4	4	13	14	5
5	5	14	15	6
6	6	15	16	7
7	7	16	17	8
8	8	17	18	9
9	10	19	20	11
10	11	20	21	12
11	12	21	22	13
12	13	22	23	14
13	14	23	24	15
14	15	24	25	16
15	16	25	26	17
16	17	26	27	18
17	19	28	29	20

18	20	29	30	21
19	21	30	31	22
20	22	31	32	23
21	23	32	33	24
22	24	33	34	25
23	25	34	35	26
24	26	35	36	27
25	28	37	38	29
26	29	38	39	30
27	30	39	40	31
28	31	40	41	32
29	32	41	42	33
30	33	42	43	34
31	34	43	44	35
32	35	44	45	36
33	37	46	47	38
34	38	47	48	39
35	39	48	49	40
36	40	49	50	41
37	41	50	51	42
38	42	51	52	43
39	43	52	53	44
40	44	53	54	45
41	46	55	56	47
42	47	56	57	48
43	48	57	58	49
44	49	58	59	50
45	50	59	60	51
46	51	60	61	52
47	52	61	62	53
48	53	62	63	54
49	55	64	65	56
50	56	65	66	57
51	57	66	67	58
52	58	67	68	59
53	59	68	69	60
54	60	69	70	61
55	61	70	71	62
56	62	71	72	63
57	64	73	74	65
58	65	74	75	66
59	66	75	76	67
60	67	76	77	68
61	68	77	78	69
62	69	78	79	70
63	70	79	80	71
64	71	80	81	72
65	73	82	83	74
66	74	83	84	75
67	75	84	85	76
68	76	85	86	77
69	77	86	87	78
70	78	87	88	79
71	79	88	89	80
72	80	89	90	81
73	82	91	92	83
74	83	92	93	84
75	84	93	94	85
76	85	94	95	86
77	86	95	96	87
78	87	96	97	88
79	88	97	98	89
80	89	98	99	90
81	91	100	101	92
82	92	101	102	93
83	93	102	103	94
84	94	103	104	95
85	95	104	105	96
86	96	105	106	97
87	97	106	107	98
88	98	107	108	99

-----MATERIAL PROPERTIES-----

--MATERIAL TYPE-- 1

KSWX	= 0.1000E+02
KRWY	= 0.5000E+01
POROSITY	= 0.3500

SM	=	0.0500
SROW	=	0.2000
ALPHA	=	5.0000
N	=	2.8000

NUMBER OF TYPE 1 BC NODES (W)	9
NUMBER OF TYPE 1 BC NODES (O)	3
NUMBER OF TYPE 1 BC NODES (G)	0
IXBC3	0

NUMBER OF TYPE 2 BC ELEMENTS (W)	0
NUMBER OF TYPE 2 BC ELEMENTS (O)	0
NUMBER OF TYPE 2 BC ELEMENTS (G)	0

NODE SCHEDULE(W)

1	6
2	5
3	4
4	3
5	2
100	10
101	9
102	8
103	7

NODE SCHEDULE(O)

45	1
54	1
63	1

BOUNDARY CONDITION SCHEDULES

0.0000	-0.1000	..SCHEDULE 1
0.0001	-0.1000	
0.0002	-0.1000	
0.0000	0.0000	..SCHEDULE 2
9999.0000	0.0000	
0.0000	1.0000	..SCHEDULE 3
9999.0000	1.0000	
0.0000	2.0000	..SCHEDULE 4
9999.0000	2.0000	
0.0000	3.0000	..SCHEDULE 5
9999.0000	3.0000	
0.0000	4.0000	..SCHEDULE 6
9999.0000	4.0000	
0.0000	0.5000	..SCHEDULE 7
9999.0000	0.5000	
0.0000	1.5000	..SCHEDULE 8
9999.0000	1.5000	
0.0000	2.5000	..SCHEDULE 9
9999.0000	2.5000	
0.0000	3.5000	..SCHEDULE 10
9999.0000	3.5000	

----TRANSPORT DATA-----

KUNIT = 2
 NO. OF SPECIES = 2
 NO. OF NODES WITH TYPE 1 BC = 0
 NO. OF ELEMENTS WITH TYPE 2 BC = 8
 NO. OF SCHEDULES DEFINING BC = 1
 EVAPORATIVE BC INDEX = 0

LONGITUDINAL DISPERSIVITY = 0.2000
 TRANSVERSE DISPERSIVITY = 0.0400
 DENSITY OF PURE WATER = 0.1000E+07
 DENSITY OF UNCONTAMINATED AIR = 0.1200E+04
 UPSTREAM WEIGHT = 1.0000
 TIME TO START UPDATE = 2.0000

----SPECIES DATA-----

----SPECIES NO:-----

EQUILIBRIUM PARTITION COEFF. BET. OIL AND WATER = 493.0000
 EQUILIBRIUM PARTITION COEFF. BET. AIR AND WATER = 0.2400
 EQUILIBRIUM PARTITION COEFF. BET. SOILD AND WATER = 0.0000
 FIRST ORDER DECAY COEFF. IN WATER = 0.0000
 FIRST ORDER DECAY COEFF. IN OIL = 0.0000
 FIRST ORDER DECAY COEFF. IN AIR = 0.0000
 FIRST ORDER DECAY COEFF. ON SOLID = 0.0000
 DIFFUSION COEFF. IN WATER = 0.0001
 DIFFUSION COEFF. IN OIL = 0.0001
 DIFFUSION COEFF. IN AIR = 0.7629
 LIQUID DENSITY OF PURE SPECIES = *****

----SPECIES NO:-----

EQUILIBRIUM PARTITION COEFF. BET. OIL AND WATER = *****
 EQUILIBRIUM PARTITION COEFF. BET. AIR AND WATER = 0.0020
 EQUILIBRIUM PARTITION COEFF. BET. SOILD AND WATER = 0.0000
 FIRST ORDER DECAY COEFF. IN WATER = 0.0000
 FIRST ORDER DECAY COEFF. IN OIL = 0.0000
 FIRST ORDER DECAY COEFF. IN AIR = 0.0000
 FIRST ORDER DECAY COEFF. ON SOLID = 0.0000
 DIFFUSION COEFF. IN WATER = 0.0000
 DIFFUSION COEFF. IN OIL = 0.0000
 DIFFUSION COEFF. IN AIR = 0.0000
 LIQUID DENSITY OF PURE SPECIES = *****

ELEMENT | SIDE | - - - SCHEDULE FOR SPECIES NO: - -
 1 2 3 4 5

1	4	1	0
2	4	1	0
3	4	1	0
4	4	1	0
5	4	1	0
6	4	1	0
7	4	1	0
8	4	1	0

TRANSPORT BOUNDARY CONDITION SCHEDULES

0.0000 0.0000 ..SCHEDULE 1

9999.0000 0.0000

*** END OF INPUT DATA ***

 NODE PROP X Z

1	1	0.0000000	0.0000000
2	1	0.0000000	1.0000000
3	1	0.0000000	2.0000000
4	1	0.0000000	3.0000000
5	1	0.0000000	4.0000000
6	1	0.0000000	5.0000000
7	1	0.0000000	6.0000000
8	1	0.0000000	7.0000000
9	1	0.0000000	8.0000000
10	1	1.0000000	0.0000000
11	1	1.0000000	1.0000000
12	1	1.0000000	2.0000000
13	1	1.0000000	3.0000000
14	1	1.0000000	4.0000000
15	1	1.0000000	5.0000000
16	1	1.0000000	6.0000000
17	1	1.0000000	7.0000000
18	1	1.0000000	8.0000000
19	1	2.0000000	0.0000000
20	1	2.0000000	1.0000000
21	1	2.0000000	2.0000000
22	1	2.0000000	3.0000000
23	1	2.0000000	4.0000000
24	1	2.0000000	5.0000000
25	1	2.0000000	6.0000000
26	1	2.0000000	7.0000000
27	1	2.0000000	8.0000000
28	1	3.0000000	0.0000000
29	1	3.0000000	1.0000000
30	1	3.0000000	2.0000000
31	1	3.0000000	3.0000000
32	1	3.0000000	4.0000000
33	1	3.0000000	5.0000000
34	1	3.0000000	6.0000000
35	1	3.0000000	7.0000000
36	1	3.0000000	8.0000000
37	1	4.0000000	0.0000000
38	1	4.0000000	1.0000000
39	1	4.0000000	2.0000000
40	1	4.0000000	3.0000000
41	1	4.0000000	4.0000000
42	1	4.0000000	5.0000000
43	1	4.0000000	6.0000000
44	1	4.0000000	7.0000000
45	1	4.0000000	8.0000000
46	1	5.0000000	0.0000000
47	1	5.0000000	1.0000000
48	1	5.0000000	2.0000000
49	1	5.0000000	3.0000000
50	1	5.0000000	4.0000000
51	1	5.0000000	5.0000000
52	1	5.0000000	6.0000000
53	1	5.0000000	7.0000000
54	1	5.0000000	8.0000000
55	1	6.0000000	0.0000000
56	1	6.0000000	1.0000000
57	1	6.0000000	2.0000000
58	1	6.0000000	3.0000000
59	1	6.0000000	4.0000000
60	1	6.0000000	5.0000000
61	1	6.0000000	6.0000000
62	1	6.0000000	7.0000000
63	1	6.0000000	8.0000000
64	1	7.0000000	0.0000000
65	1	7.0000000	1.0000000
66	1	7.0000000	2.0000000
67	1	7.0000000	3.0000000
68	1	7.0000000	4.0000000
69	1	7.0000000	5.0000000
70	1	7.0000000	6.0000000
71	1	7.0000000	7.0000000
72	1	7.0000000	8.0000000
73	1	8.0000000	0.0000000
74	1	8.0000000	1.0000000
75	1	8.0000000	2.0000000
76	1	8.0000000	3.0000000
77	1	8.0000000	4.0000000
78	1	8.0000000	5.0000000
79	1	8.0000000	6.0000000
80	1	8.0000000	7.0000000
81	1	8.0000000	8.0000000

82	1	9.0000000	0.0000000
83	1	9.0000000	1.0000000
84	1	9.0000000	2.0000000
85	1	9.0000000	3.0000000
86	1	9.0000000	4.0000000
87	1	9.0000000	5.0000000
88	1	9.0000000	6.0000000
89	1	9.0000000	7.0000000
90	1	9.0000000	8.0000000
91	1	10.0000000	0.0000000
92	1	10.0000000	1.0000000
93	1	10.0000000	2.0000000
94	1	10.0000000	3.0000000
95	1	10.0000000	4.0000000
96	1	10.0000000	5.0000000
97	1	10.0000000	6.0000000
98	1	10.0000000	7.0000000
99	1	10.0000000	8.0000000
100	1	11.0000000	0.0000000
101	1	11.0000000	1.0000000
102	1	11.0000000	2.0000000
103	1	11.0000000	3.0000000
104	1	11.0000000	4.0000000
105	1	11.0000000	5.0000000
106	1	11.0000000	6.0000000
107	1	11.0000000	7.0000000
108	1	11.0000000	8.0000000

HALF BAND WIDTH= 22

NODE |----- HEADS ---| |----- SATURATIONS -----|

HW	HO	HA	SW	SO	SA
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.... INITIAL HEADS & SATURATIONS.....

1	4.0000	3.9000	0.0000	1.0000	0.0000	0.0000
2	3.0000	2.9600	0.0000	1.0000	0.0000	0.0000
3	2.0000	1.9690	0.0000	1.0000	0.0000	0.0000
4	1.0000	0.9765	0.0000	1.0000	0.0000	0.0000
5	0.0000	0.0027	0.0000	1.0000	0.0000	0.0000
6	-1.3200	-0.4904	0.0000	0.0817	0.0000	0.9183
7	-2.0030	-0.7443	0.0000	0.0650	0.0000	0.9350
8	-3.0030	-1.1160	0.0000	0.0573	0.0000	0.9427
9	-4.0150	-1.4980	0.0000	0.0543	0.0000	0.9457
10	3.9580	3.8800	0.0000	1.0000	0.0000	0.0000
11	2.9580	2.9400	0.0000	1.0000	0.0000	0.0000
12	1.9590	1.9500	0.0000	1.0000	0.0000	0.0000
13	0.9620	0.9593	0.0000	1.0000	0.0000	0.0000
14	-0.0348	-0.0129	0.0000	0.9952	0.0003	0.0045
15	-1.2850	-0.4774	0.0000	0.0833	0.0000	0.9167
16	-2.0480	-0.7607	0.0000	0.0644	0.0000	0.9356
17	-3.0430	-1.1300	0.0000	0.0571	0.0000	0.9429
18	-4.0450	-1.5070	0.0000	0.0543	0.0000	0.9457
19	3.9150	3.8410	0.0000	1.0000	0.0000	0.0000
20	2.9160	2.9020	0.0000	1.0000	0.0000	0.0000
21	1.9180	1.9130	0.0000	1.0000	0.0000	0.0000
22	0.9229	0.9239	0.0000	1.0000	0.0000	0.0000
23	-0.0693	-0.0257	0.0000	0.9696	0.0004	0.0300
24	-1.2500	-0.4645	0.0000	0.0850	0.0000	0.9150
25	-2.0360	-0.7227	0.0000	0.0639	0.0019	0.9342
26	-2.7780	-0.8451	0.0000	0.0569	0.0050	0.9381
27	-3.6110	-1.0640	0.0000	0.0542	0.0037	0.9421
28	3.8720	3.7980	0.0000	1.0000	0.0000	0.0000
29	2.8730	2.8590	0.0000	1.0000	0.0000	0.0000
30	1.8760	1.8700	0.0000	1.0000	0.0000	0.0000
31	0.8816	0.8827	0.0000	1.0000	0.0000	0.0000
32	-0.1045	-0.0388	0.0000	0.9120	0.0006	0.0874
33	-1.2140	-0.4482	0.0000	0.0866	0.0007	0.9127
34	-1.7070	-0.3644	0.0000	0.0634	0.0406	0.8961
35	-2.1770	-0.1919	0.0000	0.0566	0.1584	0.7850
36	-2.9600	-0.3182	0.0000	0.0540	0.0647	0.8814
37	3.8280	3.7530	0.0000	1.0000	0.0000	0.0000
38	2.8290	2.8140	0.0000	1.0000	0.0000	0.0000
39	1.8320	1.8260	0.0000	1.0000	0.0000	0.0000

40	0.8377	0.8393	0.0000	1.0000	0.0000	0.0000
41	-0.1412	-0.0524	0.0000	0.8231	0.0006	0.1763
42	-1.1760	-0.4145	0.0000	0.0870	0.0059	0.9071
43	-1.5570	-0.1859	0.0000	0.0629	0.1612	0.7760
44	-2.1200	-0.1142	0.0000	0.0565	0.3640	0.5795
45	-3.0660	-0.1000	0.0000	0.0532	0.4383	0.5085
46	3.7830	3.7080	0.0000	1.0000	0.0000	0.0000
47	2.7840	2.7690	0.0000	1.0000	0.0000	0.0000
48	1.7870	1.7810	0.0000	1.0000	0.0000	0.0000
49	0.7918	0.7935	0.0000	1.0000	0.0000	0.0000
50	-0.1798	-0.0668	0.0000	0.7147	0.0006	0.2847
51	-1.1380	-0.3744	0.0000	0.0868	0.0146	0.8986
52	-1.5400	-0.1407	0.0000	0.0624	0.2604	0.6772
53	-2.1360	-0.1011	0.0000	0.0563	0.4292	0.5145
54	-3.0930	-0.1000	0.0000	0.0532	0.4384	0.5085
55	3.7380	3.6620	0.0000	1.0000	0.0000	0.0000
56	2.7390	2.7230	0.0000	1.0000	0.0000	0.0000
57	1.7410	1.7350	0.0000	1.0000	0.0000	0.0000
58	0.7449	0.7467	0.0000	1.0000	0.0000	0.0000
59	-0.2190	-0.0813	0.0000	0.6077	0.0005	0.3918
60	-1.1150	-0.3965	0.0000	0.0911	0.0054	0.9036
61	-1.6170	-0.1897	0.0000	0.0620	0.1563	0.7818
62	-2.1790	-0.1149	0.0000	0.0562	0.3612	0.5826
63	-3.1250	-0.1000	0.0000	0.0531	0.4384	0.5085
64	3.6910	3.6170	0.0000	1.0000	0.0000	0.0000
65	2.6920	2.6770	0.0000	1.0000	0.0000	0.0000
66	1.6940	1.6890	0.0000	1.0000	0.0000	0.0000
67	0.6976	0.6995	0.0000	1.0000	0.0000	0.0000
68	-0.2553	-0.0948	0.0000	0.5207	0.0005	0.4788
69	-1.1200	-0.4141	0.0000	0.0923	0.0006	0.9070
70	-1.8290	-0.3729	0.0000	0.0616	0.0402	0.8982
71	-2.2950	-0.1923	0.0000	0.0560	0.1585	0.7856
72	-3.0830	-0.3192	0.0000	0.0537	0.0646	0.8818
73	3.6440	3.5700	0.0000	1.0000	0.0000	0.0000
74	2.6450	2.6310	0.0000	1.0000	0.0000	0.0000
75	1.6470	1.6420	0.0000	1.0000	0.0000	0.0000
76	0.6501	0.6522	0.0000	1.0000	0.0000	0.0000
77	-0.2830	-0.1051	0.0000	0.4638	0.0005	0.5357
78	-1.1650	-0.4327	0.0000	0.0897	0.0000	0.9103
79	-2.2800	-0.7978	0.0000	0.0612	0.0021	0.9367
80	-2.9730	-0.8711	0.0000	0.0560	0.0053	0.9387
81	-3.7990	-1.0860	0.0000	0.0538	0.0038	0.9424
82	3.5970	3.5240	0.0000	1.0000	0.0000	0.0000
83	2.5970	2.5850	0.0000	1.0000	0.0000	0.0000
84	1.5990	1.5950	0.0000	1.0000	0.0000	0.0000
85	0.6021	0.6044	0.0000	1.0000	0.0000	0.0000
86	-0.2977	-0.1106	0.0000	0.4369	0.0003	0.5628
87	-1.2440	-0.4623	0.0000	0.0853	0.0000	0.9147
88	-2.4070	-0.8942	0.0000	0.0608	0.0000	0.9392
89	-3.4040	-1.2640	0.0000	0.0558	0.0000	0.9442
90	-4.4050	-1.6420	0.0000	0.0537	0.0000	0.9463
91	3.5480	3.4810	0.0000	1.0000	0.0000	0.0000
92	2.5490	2.5400	0.0000	1.0000	0.0000	0.0000
93	1.5500	1.5480	0.0000	1.0000	0.0000	0.0000
94	0.5531	0.5555	0.0000	1.0000	0.0000	0.0000
95	-0.2952	-0.1097	0.0000	0.4414	0.0003	0.5583
96	-1.3220	-0.4911	0.0000	0.0816	0.0000	0.9183
97	-2.4540	-0.9115	0.0000	0.0604	0.0000	0.9396
98	-3.4550	-1.2830	0.0000	0.0556	0.0000	0.9444
99	-4.4670	-1.6670	0.0000	0.0536	0.0000	0.9464
100	3.5000	3.4610	0.0000	1.0000	0.0000	0.0000
101	2.5000	2.5020	0.0000	1.0000	0.0000	0.0000
102	1.5000	1.5020	0.0000	1.0000	0.0000	0.0000
103	0.5000	0.5028	0.0000	1.0000	0.0000	0.0000
104	-0.2653	-0.0986	0.0000	0.4994	0.0002	0.5004
105	-1.3660	-0.5073	0.0000	0.0798	0.0001	0.9201
106	-2.4980	-0.9279	0.0000	0.0601	0.0000	0.9399
107	-3.4970	-1.2990	0.0000	0.0555	0.0000	0.9445
108	-4.5050	-1.6810	0.0000	0.0535	0.0000	0.9465

INITIAL VOLUME OF WATER = 17.0396
INITIAL VOLUME OF OIL = 1.0158

---INITIAL CONC OF SPECIES -----

NODE-|CONCENTRATIONS IN PHASE-
WATER OIL GAS SOLID

TOTAL MASS IN			
WATER	OIL	GAS	SOLID
0.3346E+00	0.7544E+06	0.8503E-02	0.0000E+00

***** END OF INITIAL CONDITIONS *****

FINAL OUTPUT AT TIME= 25.088608

NODE -|-----VELOCITIES-----|

	QW-X	QW-Y	QO-X	QO-Y	QA-X	QA-Y		
1	0.4192E+00		0.0000E+00		0.4340E-07	0.1182E-06	0.0000E+00	0.0000E+00
2	0.4152E+00		0.0000E+00		0.4316E-07	0.1182E-06	0.0000E+00	0.0000E+00
3	0.4020E+00		0.0000E+00		0.4301E-07	0.2794E-06	0.0000E+00	0.0000E+00
4	0.3751E+00		0.0000E+00		0.3029E-07	0.3320E-06	0.0000E+00	0.0000E+00
5	0.3409E+00		0.0000E+00		0.8596E-07	0.2881E-06	0.0000E+00	0.0000E+00
6	-0.9773E-06		0.1367E+01		-0.6363E-07	-0.8850E-06	0.0000E+00	0.0000E+00
7	0.3440E-06		-0.1309E-05		0.5680E-07	-0.1393E-05	0.0000E+00	0.0000E+00
8	-0.1079E-06		-0.3773E-07		-0.4951E-07	-0.1158E-05	0.0000E+00	0.0000E+00
9	-0.1035E-05		0.1448E-06		-0.3251E-06	-0.1064E-05	0.0000E+00	0.0000E+00
10	0.4192E+00		-0.2003E-02		0.4340E-07	0.1181E-06	0.0000E+00	0.0000E+00
11	0.4152E+00		-0.2003E-02		0.4316E-07	0.1181E-06	0.0000E+00	0.0000E+00
12	0.4020E+00		-0.6579E-02		0.4301E-07	0.2793E-06	0.0000E+00	0.0000E+00
13	0.3751E+00		-0.1348E-01		0.3029E-07	0.3257E-06	0.0000E+00	0.0000E+00
14	0.3409E+00		-0.1482E-01		0.8596E-07	0.3159E-06	0.0000E+00	0.0000E+00
15	-0.9773E-06		0.9417E+00		-0.6363E-07	-0.9598E-06	0.0000E+00	0.0000E+00
16	0.3440E-06		-0.9654E-06		0.5680E-07	-0.1333E-05	0.0000E+00	0.0000E+00
17	-0.1079E-06		-0.2637E-06		-0.4951E-07	-0.1211E-05	0.0000E+00	0.0000E+00
18	-0.1035E-05		-0.3187E-06		-0.3251E-06	-0.1202E-05	0.0000E+00	0.0000E+00
19	0.4226E+00		-0.3604E-02		0.1194E-06	0.1186E-06	0.0000E+00	0.0000E+00
20	0.4194E+00		-0.3604E-02		0.1205E-06	0.1186E-06	0.0000E+00	0.0000E+00
21	0.4087E+00		-0.1192E-01		0.1224E-06	0.2803E-06	0.0000E+00	0.0000E+00
22	0.3853E+00		-0.2518E-01		0.1024E-06	0.3157E-06	0.0000E+00	0.0000E+00
23	0.3079E+00		-0.2914E-01		0.6280E-07	0.2961E-06	0.0000E+00	0.0000E+00
24	-0.1046E-05		0.5021E+00		-0.1167E-06	-0.1050E-05	0.0000E+00	0.0000E+00
25	-0.2390E-05		-0.1992E-05		-0.1336E-05	-0.1942E-05	0.0000E+00	0.0000E+00
26	-0.5598E-05		-0.1868E-05		-0.4549E-05	-0.3073E-05	0.0000E+00	0.0000E+00
27	-0.7082E-05		-0.1060E-05		-0.4242E-05	-0.1775E-05	0.0000E+00	0.0000E+00
28	0.4290E+00		-0.4643E-02		0.1726E-06	0.1182E-06	0.0000E+00	0.0000E+00
29	0.4269E+00		-0.4643E-02		0.1717E-06	0.1182E-06	0.0000E+00	0.0000E+00
30	0.4205E+00		-0.1511E-01		0.1971E-06	0.2930E-06	0.0000E+00	0.0000E+00
31	0.4071E+00		-0.3179E-01		0.2066E-06	0.3204E-06	0.0000E+00	0.0000E+00
32	0.2449E+00		-0.3684E-01		0.5863E-07	0.2221E-06	0.0000E+00	0.0000E+00
33	-0.4277E-06		0.1761E+00		-0.2329E-04	-0.4536E-04	0.0000E+00	0.0000E+00
34	-0.2284E-05		-0.2966E-05		-0.2776E-03	-0.4721E-03	0.0000E+00	0.0000E+00
35	-0.2068E-05		-0.1759E-05		-0.4346E-03	-0.6820E-03	0.0000E+00	0.0000E+00
36	-0.1743E-05		-0.8981E-06		-0.3233E-04	-0.4170E-04	0.0000E+00	0.0000E+00
37	0.4374E+00		-0.5096E-02		0.2024E-06	0.1193E-06	0.0000E+00	0.0000E+00
38	0.4365E+00		-0.5096E-02		0.2046E-06	0.1193E-06	0.0000E+00	0.0000E+00
39	0.4346E+00		-0.1603E-01		0.1977E-06	0.2895E-06	0.0000E+00	0.0000E+00
40	0.4359E+00		-0.3111E-01		0.4797E-06	0.4614E-06	0.0000E+00	0.0000E+00
41	0.1671E+00		-0.3387E-01		0.8589E-06	0.3427E-08	0.0000E+00	0.0000E+00
42	-0.3320E-06		0.5902E-02		-0.7118E-03	-0.2176E-02	0.0000E+00	0.0000E+00
43	-0.3724E-06		-0.2986E-05		-0.5119E-03	0.3389E-02	0.0000E+00	0.0000E+00
44	-0.2959E-06		-0.1721E-05		-0.2024E-03	-0.2178E-02	0.0000E+00	0.0000E+00
45	0.1348E-05		-0.7608E-07		-0.1812E-03	-0.6449E-03	0.0000E+00	0.0000E+00
46	0.4468E+00		-0.5013E-02		0.2178E-06	0.1192E-06	0.0000E+00	0.0000E+00
47	0.4470E+00		-0.5013E-02		0.2177E-06	0.1192E-06	0.0000E+00	0.0000E+00
48	0.4480E+00		-0.1550E-01		0.2278E-06	0.2946E-06	0.0000E+00	0.0000E+00
49	0.4590E+00		-0.2561E-01		0.8837E-07	0.3917E-06	0.0000E+00	0.0000E+00
50	0.9717E-01		-0.2225E-01		0.6810E-04	-0.2277E-03	0.0000E+00	0.0000E+00
51	-0.3414E-06		-0.3263E-06		-0.4908E-03	-0.6604E-02	0.0000E+00	0.0000E+00
52	0.1697E-06		-0.2731E-05		-0.1255E-03	-0.4914E-02	0.0000E+00	0.0000E+00
53	0.2380E-06		-0.1687E-05		-0.3583E-04	-0.2623E-02	0.0000E+00	0.0000E+00
54	0.3180E-06		-0.3607E-07		-0.1550E-05	-0.6587E-03	0.0000E+00	0.0000E+00
55	0.4563E+00		-0.4609E-02		0.2244E-06	0.1182E-06	0.0000E+00	0.0000E+00
56	0.4571E+00		-0.4609E-02		0.2224E-06	0.1182E-06	0.0000E+00	0.0000E+00
57	0.4604E+00		-0.1386E-01		0.2466E-06	0.3067E-06	0.0000E+00	0.0000E+00
58	0.4642E+00		-0.2293E-01		0.5066E-07	0.2937E-06	0.0000E+00	0.0000E+00
59	0.4876E-01		-0.1607E-01		0.1052E-02	0.3446E-07	0.0000E+00	0.0000E+00
60	-0.4432E-06		-0.8627E-06		0.6265E-03	-0.1641E-02	0.0000E+00	0.0000E+00
61	0.4063E-06		-0.2348E-05		0.1505E-03	-0.3180E-02	0.0000E+00	0.0000E+00
62	0.3625E-06		-0.1709E-05		0.3932E-04	-0.2147E-02	0.0000E+00	0.0000E+00
63	0.2823E-06		-0.7618E-07		0.1678E-05	-0.6443E-03	0.0000E+00	0.0000E+00
64	0.4651E+00		-0.4126E-02		0.2250E-06	0.1194E-06	0.0000E+00	0.0000E+00
65	0.4661E+00		-0.4126E-02		0.2274E-06	0.1194E-06	0.0000E+00	0.0000E+00
66	0.4704E+00		-0.1171E-01		0.1478E-06	0.2668E-06	0.0000E+00	0.0000E+00
67	0.4668E+00		-0.1737E-01		0.2414E-05	0.3567E-06	0.0000E+00	0.0000E+00

68	0.2539E-01	-0.1277E-01	0.5173E-04	-0.1787E-06	0.0000E+00	0.0000E+00
69	-0.1014E-05	-0.3569E-05	0.4759E-03	-0.3702E-04	0.0000E+00	0.0000E+00
70	0.9755E-06	-0.1717E-05	0.4894E-03	-0.4319E-03	0.0000E+00	0.0000E+00
71	0.9241E-06	-0.1735E-05	0.1999E-03	-0.6742E-03	0.0000E+00	0.0000E+00
72	-0.6285E-06	-0.8524E-06	0.1840E-03	-0.4026E-04	0.0000E+00	0.0000E+00
73	0.4730E+00	-0.3526E-02	0.2191E-06	0.1191E-06	0.0000E+00	0.0000E+00
74	0.4742E+00	-0.3526E-02	0.2186E-06	0.1191E-06	0.0000E+00	0.0000E+00
75	0.4766E+00	-0.1050E-01	0.2583E-06	0.2867E-06	0.0000E+00	0.0000E+00
76	0.4726E+00	-0.1728E-01	0.2527E-06	0.3539E-06	0.0000E+00	0.0000E+00
77	0.1118E-01	-0.1149E-01	0.9638E-07	-0.1933E-06	0.0000E+00	0.0000E+00
78	-0.1166E-05	-0.1072E-04	0.1051E-04	-0.1389E-05	0.0000E+00	0.0000E+00
79	0.2935E-05	-0.1839E-06	0.2705E-03	-0.1742E-05	0.0000E+00	0.0000E+00
80	0.2684E-05	-0.1860E-05	0.4337E-03	-0.3133E-05	0.0000E+00	0.0000E+00
81	0.2390E-05	-0.9990E-06	0.3142E-04	-0.1777E-05	0.0000E+00	0.0000E+00
82	0.4795E+00	-0.2636E-02	0.1951E-06	0.1236E-06	0.0000E+00	0.0000E+00
83	0.4813E+00	-0.2636E-02	0.2040E-06	0.1236E-06	0.0000E+00	0.0000E+00
84	0.4838E+00	-0.9238E-02	0.2244E-06	0.2969E-06	0.0000E+00	0.0000E+00
85	0.4791E+00	-0.1889E-01	0.2391E-06	0.3613E-06	0.0000E+00	0.0000E+00
86	0.4054E-02	-0.1306E-01	0.2621E-07	-0.2998E-06	0.0000E+00	0.0000E+00
87	0.2665E-06	-0.1202E-04	0.3494E-07	-0.1385E-05	0.0000E+00	0.0000E+00
88	0.3868E-05	0.1656E-04	0.1852E-05	-0.8335E-06	0.0000E+00	0.0000E+00
89	0.7104E-05	-0.2423E-06	0.5422E-05	-0.1213E-05	0.0000E+00	0.0000E+00
90	0.8306E-05	-0.3982E-06	0.4805E-05	-0.1216E-05	0.0000E+00	0.0000E+00
91	0.4844E+00	-0.1546E-02	0.1342E-06	0.1343E-06	0.0000E+00	0.0000E+00
92	0.4865E+00	-0.1546E-02	0.1556E-06	0.1343E-06	0.0000E+00	0.0000E+00
93	0.4950E+00	-0.5005E-02	0.2054E-06	0.3218E-06	0.0000E+00	0.0000E+00
94	0.4901E+00	-0.2045E-01	0.2448E-06	0.3809E-06	0.0000E+00	0.0000E+00
95	-0.2450E-03	-0.1925E-01	-0.1807E-08	-0.4231E-06	0.0000E+00	0.0000E+00
96	0.1467E-05	-0.1018E-04	0.2836E-07	-0.1370E-05	0.0000E+00	0.0000E+00
97	0.6493E-06	0.1716E-04	0.1268E-06	-0.7843E-06	0.0000E+00	0.0000E+00
98	0.1194E-05	0.2996E-07	0.2593E-06	-0.1146E-05	0.0000E+00	0.0000E+00
99	0.2278E-05	0.1440E-06	0.5994E-06	-0.1046E-05	0.0000E+00	0.0000E+00
100	0.4867E+00	0.0000E+00	0.5587E-07	0.1090E-06	0.0000E+00	0.0000E+00
101	0.4898E+00	0.0000E+00	0.5317E-08	0.1090E-06	0.0000E+00	0.0000E+00
102	0.4999E+00	0.0000E+00	0.1966E-06	0.4175E-06	0.0000E+00	0.0000E+00
103	0.5387E+00	0.0000E+00	0.2668E-06	0.4160E-06	0.0000E+00	0.0000E+00
104	-0.1119E-01	-0.4811E-01	-0.5346E-07	-0.5832E-06	0.0000E+00	0.0000E+00
105	0.2720E-05	-0.6136E-05	0.5821E-07	-0.1314E-05	0.0000E+00	0.0000E+00
106	0.3748E-06	0.1410E-04	0.6933E-07	-0.7787E-06	0.0000E+00	0.0000E+00
107	0.3878E-06	0.3646E-07	0.7376E-07	-0.1144E-05	0.0000E+00	0.0000E+00
108	0.4176E-06	0.1589E-06	0.8426E-07	-0.1041E-05	0.0000E+00	0.0000E+00

NODE |----- HEADS ---| |----- SATURATIONS -----|

	HW	HO	HA	SW	SO	SA
1	4.0000	3.7397	0.0000	1.0000	0.0000	0.0000
2	3.0000	2.8604	0.0000	1.0000	0.0000	0.0000
3	2.0000	1.9166	0.0000	1.0000	0.0000	0.0000
4	1.0000	0.9517	0.0000	1.0000	0.0000	0.0000
5	0.0000	0.0045	0.0000	0.9999	0.0001	0.0000
6	-1.2748	-0.4735	0.0000	0.0837	0.0001	0.9162
7	-2.0130	-0.7484	0.0000	0.0649	0.0000	0.9351
8	-3.0055	-1.1171	0.0000	0.0572	0.0000	0.9428
9	-4.0344	-1.5234	0.0000	0.0543	0.0000	0.9457
10	3.9581	3.7310	0.0000	1.0000	0.0000	0.0000
11	2.9585	2.8517	0.0000	1.0000	0.0000	0.0000
12	1.9598	1.9080	0.0000	1.0000	0.0000	0.0000
13	0.9625	0.9457	0.0000	1.0000	0.0000	0.0000
14	-0.0343	-0.0127	0.0000	0.9954	0.0003	0.0043
15	-1.2405	-0.4608	0.0000	0.0853	0.0001	0.9145
16	-2.0474	-0.7597	0.0000	0.0644	0.0000	0.9355
17	-2.9947	-1.1072	0.0000	0.0572	0.0001	0.9426
18	-3.9309	-1.4584	0.0000	0.0545	0.0000	0.9455
19	3.9158	3.7071	0.0000	1.0000	0.0000	0.0000
20	2.9165	2.8276	0.0000	1.0000	0.0000	0.0000
21	1.9189	1.8835	0.0000	1.0000	0.0000	0.0000
22	0.9240	0.9252	0.0000	1.0000	0.0000	0.0000
23	-0.0680	-0.0252	0.0000	0.9701	0.0013	0.0285
24	-1.2069	-0.4374	0.0000	0.0862	0.0028	0.9111
25	-1.8084	-0.4925	0.0000	0.0639	0.0176	0.9185
26	-2.4349	-0.4878	0.0000	0.0569	0.0252	0.9180
27	-3.2228	-0.6100	0.0000	0.0540	0.0174	0.9285
28	3.8729	3.6726	0.0000	1.0000	0.0000	0.0000
29	2.8739	2.7933	0.0000	1.0000	0.0000	0.0000
30	1.8769	1.8441	0.0000	1.0000	0.0000	0.0000
31	0.8832	0.8839	0.0000	1.0000	0.0000	0.0000
32	-0.1018	-0.0370	0.0000	0.9133	0.0092	0.0775

33	-1.1732	-0.2884	0.0000	0.0783	0.0534	0.8684
34	-1.5799	-0.2311	0.0000	0.0633	0.1069	0.8298
35	-2.2281	-0.2188	0.0000	0.0565	0.1255	0.8180
36	-3.0484	-0.3309	0.0000	0.0538	0.0603	0.8860
37	3.8292	3.6321	0.0000	1.0000	0.0000	0.0000
38	2.8302	2.7524	0.0000	1.0000	0.0000	0.0000
39	1.8334	1.8045	0.0000	1.0000	0.0000	0.0000
40	0.8396	0.7880	0.0000	1.0000	0.0000	0.0000
41	-0.1357	-0.0454	0.0000	0.8152	0.0571	0.1277
42	-1.1400	-0.1732	0.0000	0.0741	0.1716	0.7542
43	-1.5427	-0.1678	0.0000	0.0628	0.1933	0.7439
44	-2.1985	-0.1808	0.0000	0.0564	0.1759	0.7677
45	-3.1833	-0.2194	0.0000	0.0532	0.1282	0.8186
46	3.7845	3.5885	0.0000	1.0000	0.0000	0.0000
47	2.7855	2.7088	0.0000	1.0000	0.0000	0.0000
48	1.7886	1.7590	0.0000	1.0000	0.0000	0.0000
49	0.7937	0.7703	0.0000	1.0000	0.0000	0.0000
50	-0.1711	-0.0528	0.0000	0.6892	0.1318	0.1790
51	-1.1058	-0.1457	0.0000	0.0744	0.2339	0.6916
52	-1.5597	-0.1573	0.0000	0.0624	0.2164	0.7212
53	-2.2223	-0.1752	0.0000	0.0563	0.1858	0.7580
54	-3.2151	-0.2185	0.0000	0.0532	0.1292	0.8177
55	3.7389	3.5437	0.0000	1.0000	0.0000	0.0000
56	2.7398	2.6644	0.0000	1.0000	0.0000	0.0000
57	1.7426	1.7097	0.0000	1.0000	0.0000	0.0000
58	0.7473	0.7602	0.0000	0.9990	0.0010	0.0000
59	-0.2096	-0.0734	0.0000	0.6110	0.0542	0.3348
60	-1.0700	-0.1808	0.0000	0.0780	0.1543	0.7677
61	-1.6003	-0.1699	0.0000	0.0619	0.1901	0.7480
62	-2.2585	-0.1813	0.0000	0.0561	0.1753	0.7686
63	-3.2433	-0.2195	0.0000	0.0531	0.1282	0.8187
64	3.6924	3.4987	0.0000	1.0000	0.0000	0.0000
65	2.6932	2.6189	0.0000	1.0000	0.0000	0.0000
66	1.6955	1.6801	0.0000	1.0000	0.0000	0.0000
67	0.6990	0.7054	0.0000	0.9999	0.0001	0.0000
68	-0.2436	-0.0899	0.0000	0.5419	0.0093	0.4488
69	-1.0412	-0.2858	0.0000	0.0875	0.0454	0.8671
70	-1.6978	-0.2348	0.0000	0.0615	0.1055	0.8331
71	-2.3509	-0.2195	0.0000	0.0558	0.1255	0.8187
72	-3.1804	-0.3329	0.0000	0.0535	0.0599	0.8866
73	3.6451	3.4548	0.0000	1.0000	0.0000	0.0000
74	2.6458	2.5752	0.0000	1.0000	0.0000	0.0000
75	1.6479	1.6284	0.0000	1.0000	0.0000	0.0000
76	0.6513	0.6549	0.0000	1.0000	0.0000	0.0000
77	-0.2687	-0.0998	0.0000	0.4891	0.0034	0.5075
78	-1.0281	-0.3762	0.0000	0.0984	0.0026	0.8990
79	-1.9913	-0.5113	0.0000	0.0612	0.0182	0.9205
80	-2.6193	-0.4920	0.0000	0.0558	0.0257	0.9184
81	-3.4195	-0.6133	0.0000	0.0536	0.0177	0.9287
82	3.5971	3.4158	0.0000	1.0000	0.0000	0.0000
83	2.5976	2.5343	0.0000	1.0000	0.0000	0.0000
84	1.5995	1.5836	0.0000	1.0000	0.0000	0.0000
85	0.6033	0.6070	0.0000	1.0000	0.0000	0.0000
86	-0.2828	-0.1051	0.0000	0.4638	0.0007	0.5355
87	-1.0311	-0.3832	0.0000	0.0994	0.0000	0.9006
88	-2.3781	-0.8818	0.0000	0.0610	0.0001	0.9389
89	-3.3297	-1.2288	0.0000	0.0560	0.0001	0.9439
90	-4.2500	-1.5744	0.0000	0.0539	0.0000	0.9461
91	3.5487	3.3890	0.0000	1.0000	0.0000	0.0000
92	2.5490	2.5032	0.0000	1.0000	0.0000	0.0000
93	1.5500	1.5425	0.0000	1.0000	0.0000	0.0000
94	0.5541	0.5581	0.0000	1.0000	0.0000	0.0000
95	-0.2818	-0.1047	0.0000	0.4663	0.0003	0.5335
96	-1.0465	-0.3888	0.0000	0.0980	0.0000	0.9019
97	-2.4431	-0.9071	0.0000	0.0605	0.0000	0.9395
98	-3.4491	-1.2806	0.0000	0.0556	0.0000	0.9443
99	-4.4779	-1.6943	0.0000	0.0536	0.0000	0.9464
100	3.5000	3.3778	0.0000	1.0000	0.0000	0.0000
101	2.5000	2.5022	0.0000	1.0000	0.0000	0.0000
102	1.5000	1.5032	0.0000	1.0000	0.0000	0.0000
103	0.5000	0.5047	0.0000	0.9999	0.0001	0.0000
104	-0.2531	-0.0940	0.0000	0.5252	0.0009	0.4739
105	-1.0779	-0.4005	0.0000	0.0953	0.0003	0.9044
106	-2.4806	-0.9210	0.0000	0.0602	0.0000	0.9398
107	-3.4878	-1.2954	0.0000	0.0555	0.0000	0.9445
108	-4.5196	-1.7111	0.0000	0.0535	0.0000	0.9465

FINAL VOLUME OF WATER = 17.0679
 FINAL VOLUME OF OIL = 1.0120

TOTAL ITERATIONS 327
TOTAL TIME STEPS 327

***** RESULTS OF TRANSPORT *****

NODE-|CONCENTRATIONS IN PHASE-
WATER OIL GAS SOLID

SPECIES NUMBER = 1

1	0.4086E-03	0.0000E+00	0.0000E+00	0.0000E+00
2	0.1754E-02	0.0000E+00	0.0000E+00	0.0000E+00
3	0.2040E-01	0.0000E+00	0.0000E+00	0.0000E+00
4	0.1983E+00	0.0000E+00	0.0000E+00	0.0000E+00
5	0.1120E+01	0.0000E+00	0.0000E+00	0.0000E+00
6	0.1361E+01	0.0000E+00	0.3266E+00	0.0000E+00
7	0.6695E+01	0.0000E+00	0.1607E+01	0.0000E+00
8	0.6556E+02	0.0000E+00	0.1573E+02	0.0000E+00
9	0.8976E+02	0.0000E+00	0.2154E+02	0.0000E+00
10	0.2163E-02	0.0000E+00	0.0000E+00	0.0000E+00
11	0.3079E-02	0.0000E+00	0.0000E+00	0.0000E+00
12	0.4816E-01	0.0000E+00	0.0000E+00	0.0000E+00
13	0.5330E+00	0.0000E+00	0.0000E+00	0.0000E+00
14	0.4518E+01	0.0000E+00	0.1084E+01	0.0000E+00
15	0.6243E+01	0.0000E+00	0.1498E+01	0.0000E+00
16	0.8732E+01	0.0000E+00	0.2096E+01	0.0000E+00
17	0.8939E+02	0.0000E+00	0.2145E+02	0.0000E+00
18	0.1135E+03	0.0000E+00	0.2725E+02	0.0000E+00
19	0.1739E-01	0.0000E+00	0.0000E+00	0.0000E+00
20	0.4171E-03	0.0000E+00	0.0000E+00	0.0000E+00
21	0.1478E+00	0.0000E+00	0.0000E+00	0.0000E+00
22	0.1675E+01	0.0000E+00	0.0000E+00	0.0000E+00
23	0.1647E+02	0.0000E+00	0.3954E+01	0.0000E+00
24	0.2443E+02	0.1204E+05	0.5863E+01	0.0000E+00
25	0.8065E+02	0.3976E+05	0.1936E+02	0.0000E+00
26	0.1654E+03	0.8156E+05	0.3970E+02	0.0000E+00
27	0.1632E+03	0.8047E+05	0.3918E+02	0.0000E+00
28	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
29	0.1397E+00	0.0000E+00	0.0000E+00	0.0000E+00
30	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
31	0.5898E+01	0.0000E+00	0.0000E+00	0.0000E+00
32	0.4600E+02	0.2268E+05	0.1104E+02	0.0000E+00
33	0.1347E+03	0.6639E+05	0.3232E+02	0.0000E+00
34	0.1781E+03	0.8782E+05	0.4275E+02	0.0000E+00
35	0.1778E+03	0.8765E+05	0.4267E+02	0.0000E+00
36	0.1789E+03	0.8820E+05	0.4294E+02	0.0000E+00
37	0.1762E+00	0.0000E+00	0.0000E+00	0.0000E+00
38	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
39	0.1514E+01	0.0000E+00	0.0000E+00	0.0000E+00
40	0.7630E+01	0.0000E+00	0.0000E+00	0.0000E+00
41	0.1478E+03	0.7287E+05	0.3547E+02	0.0000E+00
42	0.1812E+03	0.8932E+05	0.4348E+02	0.0000E+00
43	0.1774E+03	0.8744E+05	0.4257E+02	0.0000E+00
44	0.1780E+03	0.8776E+05	0.4272E+02	0.0000E+00
45	0.1778E+03	0.8767E+05	0.4268E+02	0.0000E+00
46	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
47	0.6265E+00	0.0000E+00	0.0000E+00	0.0000E+00
48	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
49	0.3002E+02	0.0000E+00	0.0000E+00	0.0000E+00
50	0.1797E+03	0.8859E+05	0.4313E+02	0.0000E+00
51	0.1768E+03	0.8716E+05	0.4243E+02	0.0000E+00
52	0.1781E+03	0.8778E+05	0.4273E+02	0.0000E+00
53	0.1778E+03	0.8767E+05	0.4268E+02	0.0000E+00
54	0.1779E+03	0.8769E+05	0.4269E+02	0.0000E+00
55	0.1306E+00	0.0000E+00	0.0000E+00	0.0000E+00
56	0.4056E+00	0.0000E+00	0.0000E+00	0.0000E+00
57	0.1074E+01	0.0000E+00	0.0000E+00	0.0000E+00
58	0.4291E+02	0.2115E+05	0.0000E+00	0.0000E+00
59	0.1797E+03	0.8860E+05	0.4313E+02	0.0000E+00
60	0.1794E+03	0.8846E+05	0.4307E+02	0.0000E+00
61	0.1778E+03	0.8767E+05	0.4268E+02	0.0000E+00
62	0.1778E+03	0.8768E+05	0.4268E+02	0.0000E+00
63	0.1779E+03	0.8772E+05	0.4271E+02	0.0000E+00
64	0.2821E+00	0.0000E+00	0.0000E+00	0.0000E+00
65	0.6066E-01	0.0000E+00	0.0000E+00	0.0000E+00
66	0.3535E+01	0.0000E+00	0.0000E+00	0.0000E+00
67	0.5018E+02	0.0000E+00	0.0000E+00	0.0000E+00

68	0.1657E+03	0.8168E+05	0.3976E+02	0.0000E+00
69	0.1777E+03	0.8762E+05	0.4265E+02	0.0000E+00
70	0.1768E+03	0.8718E+05	0.4244E+02	0.0000E+00
71	0.1778E+03	0.8767E+05	0.4268E+02	0.0000E+00
72	0.1779E+03	0.8769E+05	0.4269E+02	0.0000E+00
73	0.3233E+00	0.0000E+00	0.0000E+00	0.0000E+00
74	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
75	0.6116E+01	0.0000E+00	0.0000E+00	0.0000E+00
76	0.5632E+02	0.0000E+00	0.0000E+00	0.0000E+00
77	0.1356E+03	0.0000E+00	0.3255E+02	0.0000E+00
78	0.1653E+03	0.8147E+05	0.3966E+02	0.0000E+00
79	0.1745E+03	0.8601E+05	0.4187E+02	0.0000E+00
80	0.1763E+03	0.8694E+05	0.4232E+02	0.0000E+00
81	0.1767E+03	0.8709E+05	0.4240E+02	0.0000E+00
82	0.3442E+00	0.0000E+00	0.0000E+00	0.0000E+00
83	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
84	0.9120E+01	0.0000E+00	0.0000E+00	0.0000E+00
85	0.5930E+02	0.0000E+00	0.0000E+00	0.0000E+00
86	0.1187E+03	0.0000E+00	0.2848E+02	0.0000E+00
87	0.1454E+03	0.0000E+00	0.3491E+02	0.0000E+00
88	0.1639E+03	0.0000E+00	0.3934E+02	0.0000E+00
89	0.1710E+03	0.0000E+00	0.4105E+02	0.0000E+00
90	0.1705E+03	0.0000E+00	0.4092E+02	0.0000E+00
91	0.2995E+00	0.0000E+00	0.0000E+00	0.0000E+00
92	0.3389E-01	0.0000E+00	0.0000E+00	0.0000E+00
93	0.1154E+02	0.0000E+00	0.0000E+00	0.0000E+00
94	0.6081E+02	0.0000E+00	0.0000E+00	0.0000E+00
95	0.1099E+03	0.0000E+00	0.2637E+02	0.0000E+00
96	0.1331E+03	0.0000E+00	0.3196E+02	0.0000E+00
97	0.1487E+03	0.0000E+00	0.3568E+02	0.0000E+00
98	0.1579E+03	0.0000E+00	0.3790E+02	0.0000E+00
99	0.1609E+03	0.0000E+00	0.3861E+02	0.0000E+00
100	0.2448E+00	0.0000E+00	0.0000E+00	0.0000E+00
101	0.1237E+00	0.0000E+00	0.0000E+00	0.0000E+00
102	0.1234E+02	0.0000E+00	0.0000E+00	0.0000E+00
103	0.6121E+02	0.0000E+00	0.0000E+00	0.0000E+00
104	0.1079E+03	0.0000E+00	0.2590E+02	0.0000E+00
105	0.1282E+03	0.0000E+00	0.3077E+02	0.0000E+00
106	0.1439E+03	0.0000E+00	0.3453E+02	0.0000E+00
107	0.1533E+03	0.0000E+00	0.3680E+02	0.0000E+00
108	0.1566E+03	0.0000E+00	0.3758E+02	0.0000E+00

TOTAL MASS IN

WATER OIL GAS SOLID
0.5090E+03 0.8736E+05 0.4345E+03 0.0000E+00

SPECIES NUMBER = 2

1	0.2692E-03	0.0000E+00	0.0000E+00	0.0000E+00
2	0.1017E-02	0.0000E+00	0.0000E+00	0.0000E+00
3	0.5936E-03	0.0000E+00	0.0000E+00	0.0000E+00
4	0.9402E-02	0.0000E+00	0.0000E+00	0.0000E+00
5	0.3570E-02	0.0000E+00	0.0000E+00	0.0000E+00
6	0.2407E+00	0.0000E+00	0.4814E-03	0.0000E+00
7	0.4893E+00	0.0000E+00	0.9785E-03	0.0000E+00
8	0.5020E+00	0.0000E+00	0.1004E-02	0.0000E+00
9	0.4151E+00	0.0000E+00	0.8302E-03	0.0000E+00
10	0.3112E-02	0.0000E+00	0.0000E+00	0.0000E+00
11	0.2099E-03	0.0000E+00	0.0000E+00	0.0000E+00
12	0.2469E-01	0.0000E+00	0.0000E+00	0.0000E+00
13	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
14	0.2656E+00	0.0000E+00	0.5312E-03	0.0000E+00
15	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
16	0.1008E+00	0.0000E+00	0.2016E-03	0.0000E+00
17	0.6104E-01	0.0000E+00	0.1221E-03	0.0000E+00
18	0.1205E+00	0.0000E+00	0.2410E-03	0.0000E+00
19	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
20	0.2040E-01	0.0000E+00	0.0000E+00	0.0000E+00
21	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
22	0.3916E+00	0.0000E+00	0.0000E+00	0.0000E+00
23	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
24	0.4633E+00	0.4633E+06	0.9266E-03	0.0000E+00
25	0.7895E+00	0.7895E+06	0.1579E-02	0.0000E+00
26	0.7501E+00	0.7501E+06	0.1500E-02	0.0000E+00
27	0.7511E+00	0.7511E+06	0.1502E-02	0.0000E+00

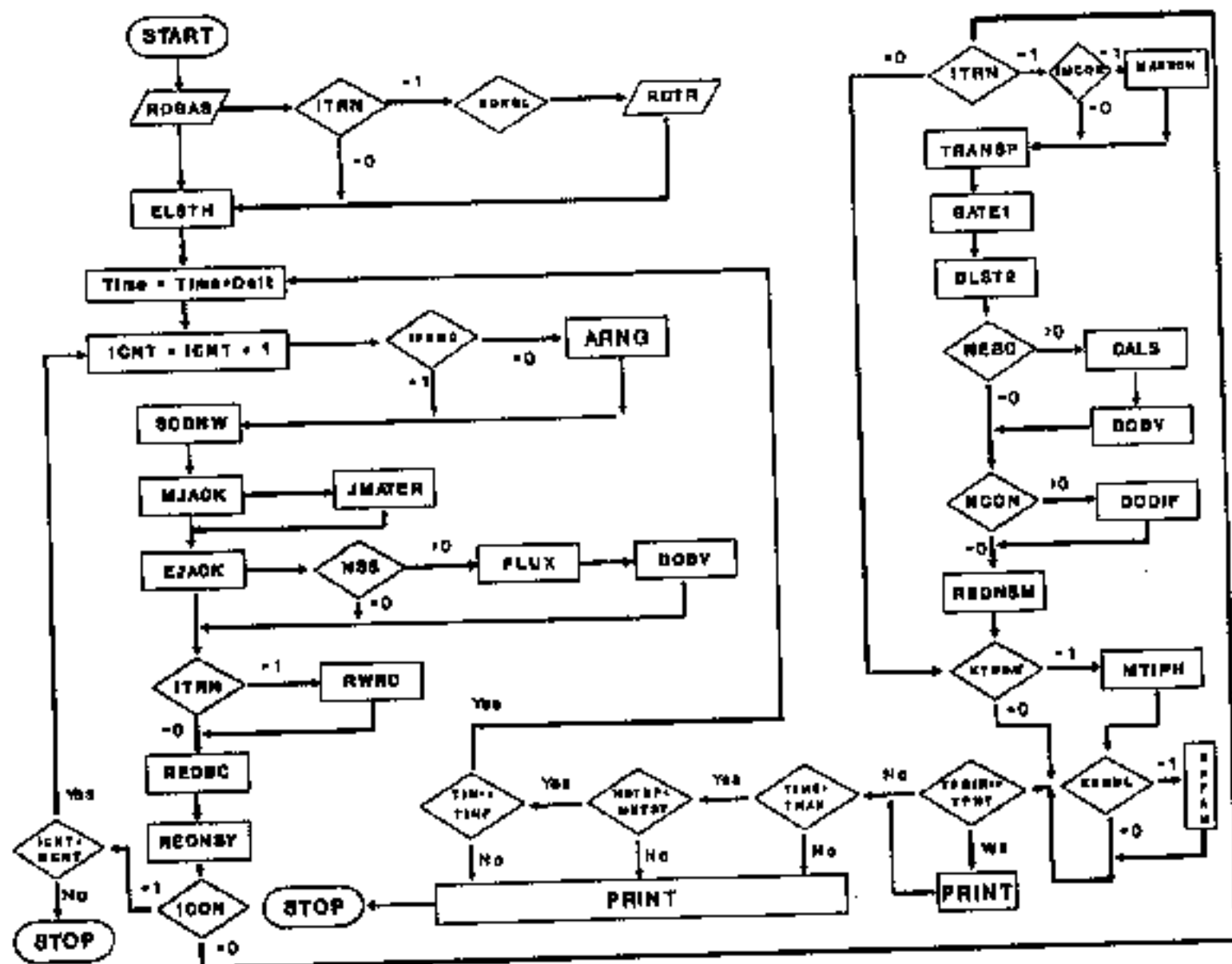
28	0.8927E-02	0.0000E+00	0.0000E+00	0.0000E+00
29	0.2759E-02	0.0000E+00	0.0000E+00	0.0000E+00
30	0.7571E-01	0.0000E+00	0.0000E+00	0.0000E+00
31	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
32	0.5160E+00	0.5160E+06	0.1032E-02	0.0000E+00
33	0.7644E+00	0.7644E+06	0.1529E-02	0.0000E+00
34	0.7442E+00	0.7442E+06	0.1488E-02	0.0000E+00
35	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
36	0.7438E+00	0.7438E+06	0.1488E-02	0.0000E+00
37	0.5189E-02	0.0000E+00	0.0000E+00	0.0000E+00
38	0.1095E-01	0.0000E+00	0.0000E+00	0.0000E+00
39	0.4728E-01	0.0000E+00	0.0000E+00	0.0000E+00
40	0.3296E-01	0.0000E+00	0.0000E+00	0.0000E+00
41	0.7583E+00	0.7583E+06	0.1517E-02	0.0000E+00
42	0.7428E+00	0.7428E+06	0.1486E-02	0.0000E+00
43	0.7445E+00	0.7445E+06	0.1489E-02	0.0000E+00
44	0.7442E+00	0.7442E+06	0.1488E-02	0.0000E+00
45	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
46	0.2833E-02	0.0000E+00	0.0000E+00	0.0000E+00
47	0.1747E-01	0.0000E+00	0.0000E+00	0.0000E+00
48	0.1151E-01	0.0000E+00	0.0000E+00	0.0000E+00
49	0.1522E+00	0.0000E+00	0.0000E+00	0.0000E+00
50	0.7435E+00	0.7435E+06	0.1487E-02	0.0000E+00
51	0.7448E+00	0.7448E+06	0.1490E-02	0.0000E+00
52	0.7442E+00	0.7442E+06	0.1488E-02	0.0000E+00
53	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
54	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
55	0.5655E-02	0.0000E+00	0.0000E+00	0.0000E+00
56	0.1251E-01	0.0000E+00	0.0000E+00	0.0000E+00
57	0.2329E-01	0.0000E+00	0.0000E+00	0.0000E+00
58	0.7950E-01	0.7950E+05	0.0000E+00	0.0000E+00
59	0.7435E+00	0.7435E+06	0.1487E-02	0.0000E+00
60	0.7436E+00	0.7436E+06	0.1487E-02	0.0000E+00
61	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
62	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
63	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
64	0.6608E-02	0.0000E+00	0.0000E+00	0.0000E+00
65	0.1068E-01	0.0000E+00	0.0000E+00	0.0000E+00
66	0.2964E-01	0.0000E+00	0.0000E+00	0.0000E+00
67	0.3954E-01	0.0000E+00	0.0000E+00	0.0000E+00
68	0.6200E+00	0.6200E+06	0.1240E-02	0.0000E+00
69	0.7444E+00	0.7444E+06	0.1489E-02	0.0000E+00
70	0.7448E+00	0.7448E+06	0.1490E-02	0.0000E+00
71	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
72	0.7443E+00	0.7443E+06	0.1489E-02	0.0000E+00
73	0.7669E-02	0.0000E+00	0.0000E+00	0.0000E+00
74	0.8630E-02	0.0000E+00	0.0000E+00	0.0000E+00
75	0.3527E-01	0.0000E+00	0.0000E+00	0.0000E+00
76	0.8822E-02	0.0000E+00	0.0000E+00	0.0000E+00
77	0.1254E+00	0.0000E+00	0.2509E-03	0.0000E+00
78	0.7548E+00	0.7548E+06	0.1510E-02	0.0000E+00
79	0.7459E+00	0.7459E+06	0.1492E-02	0.0000E+00
80	0.7450E+00	0.7450E+06	0.1490E-02	0.0000E+00
81	0.7449E+00	0.7449E+06	0.1490E-02	0.0000E+00
82	0.4267E-02	0.0000E+00	0.0000E+00	0.0000E+00
83	0.1618E-01	0.0000E+00	0.0000E+00	0.0000E+00
84	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
85	0.1639E+00	0.0000E+00	0.0000E+00	0.0000E+00
86	0.1307E+00	0.0000E+00	0.2614E-03	0.0000E+00
87	0.6823E+00	0.0000E+00	0.1365E-02	0.0000E+00
88	0.7535E+00	0.0000E+00	0.1507E-02	0.0000E+00
89	0.7449E+00	0.0000E+00	0.1490E-02	0.0000E+00
90	0.7470E+00	0.0000E+00	0.1494E-02	0.0000E+00
91	0.8855E-02	0.0000E+00	0.0000E+00	0.0000E+00
92	0.7154E-02	0.0000E+00	0.0000E+00	0.0000E+00
93	0.3209E-01	0.0000E+00	0.0000E+00	0.0000E+00
94	0.1682E-01	0.0000E+00	0.0000E+00	0.0000E+00
95	0.8270E+00	0.0000E+00	0.1654E-02	0.0000E+00
96	0.7555E+00	0.0000E+00	0.1511E-02	0.0000E+00
97	0.7452E+00	0.0000E+00	0.1490E-02	0.0000E+00
98	0.7471E+00	0.0000E+00	0.1494E-02	0.0000E+00
99	0.7459E+00	0.0000E+00	0.1492E-02	0.0000E+00
100	0.7023E-02	0.0000E+00	0.0000E+00	0.0000E+00
101	0.1071E-01	0.0000E+00	0.0000E+00	0.0000E+00
102	0.2120E-01	0.0000E+00	0.0000E+00	0.0000E+00
103	0.3906E-01	0.0000E+00	0.0000E+00	0.0000E+00
104	0.7671E+00	0.0000E+00	0.1534E-02	0.0000E+00
105	0.7267E+00	0.0000E+00	0.1453E-02	0.0000E+00
106	0.7352E+00	0.0000E+00	0.1470E-02	0.0000E+00
107	0.7419E+00	0.0000E+00	0.1484E-02	0.0000E+00
108	0.7479E+00	0.0000E+00	0.1496E-02	0.0000E+00

TOTAL MASS IN

WATER	OIL	GAS	SOLID
0.2229E+01	0.7511E+06	0.1637E-01	0.0000E+00

END OF SIMULATION RUN

APPENDIX D. FLOW CHART FOR PROGRAM



APPENDIX E: DESCRIPTION OF SUBROUTINES

ARNG	Arranges active nodes for ASD options in ascending order
BMASS	Computes volume of fluids in various phases from saturations for Cartesian domain
BONEL	Sorts out elements on the boundary of the domain
CALS	Returns the local and the global node number of nodes given the element number and the side for assigning type-3 transport boundary conditions
CONN	Gives numbers of connected nodes for any node in the domain
DENU	Updates fluid densities from fluid composition
DLST2	Computes element stiffness matrix for transport problem
DMASS	Computes the mass for each species in different phases
DOBV	Computes type-3 boundary conditions for transport problem for an element side from the assigned schedule
DOBW	Computes fluid fluxes for type-2 flow boundary conditions for an element side from the assigned schedule
DODIF	Imposes type-1 boundary conditions for transport problem
DVELO	Computes fluid velocities for water, oil and gas phases at nodes in the domain
EJACK	Evaluates element stiffness matrix for flow problem
ELST4	Assigns area for Cartesian problem or volume for radial problem to each node in the domain
FLUX	Calls DOBW for an element with type-2 flow boundary conditions and modifies the element stiffness matrix accordingly with the information returned from DOBW
GASX	Assigns the prescribed minimum gas pressure to nodes with total liquid saturation = 1
GATE1	Evaluates element properties required in DLST2
JMATER problem	Computes nodal properties required in the element stiffness matrix for flow problem

MASSCH	Computes mass injection rates for components in the transport module
MJACK	Assigns nodal properties computed in JMATER for each node of the element to the relevant arrays and sends to EJACK
MTIPH	Computes interphase mass transfer terms
RDGAS	Reads input data for flow module
RDTR	Reads input data for transport module
REDBC	Imposes boundary conditions for the Newton-Raphson scheme
REDNSY	Solves the global assembled equations
RMASS	Computes the volume of fluids in various phases in a radial domain
RWRO	Modifies load vector in the fluid flow module to account for interphase transfer
SODNW	Assigns values of type-1 flow boundary conditions to nodes from the corresponding schedules
TRANSP	Main control subroutine for the transport module
UPFAM	Computes nonequilibrium interphase partition coefficients
UPWIND2	Computes the upstream weighting for the flow module
WRTR	Prints output for the transport module
XYZ	Computes nodal coordinates and node numbers for each element in the domain

APPENDIX F DEFINITIONS OF IMPORTANT VARIABLES

ABSA	Absolute convergence limit for all liquid heads
ABSC	Absolute convergence limit for concentration of species in water phase under nonequilibrium mass transfer conditions
AKWX	Conductivity of water in x-direction
AKWY	Conductivity of water in y-direction
AKOX	Conductivity of oil in x-direction
AKOY	Conductivity of oil in y-direction
AKAX	Conductivity of gas in x-direction
AKAY	Conductivity of gas in y-direction
ALM	Gas compressibility
A	Global stiffness matrix
B	Global load vector in the flow module
AMASS	Accumulated mass for species in various phases
ACN	Boundary condition schedules in the transport module
ACDF	Node numbers connected to nodes in the domain (connectivity matrix)
BRN	Temporary storage for material properties in the flow module
CFn	Temporary storage for element material properties required in the evaluation of the element stiffness matrix in subroutine EJACK (n=1, 2, 3, 4, 41, 42, 44, 45, N41, N42, N44, N45)
CHU	Array to store fluid pressure heads at which derivatives in the Newton-Raphson scheme are evaluated
CHA	Array to store fluid pressure heads at start of the time step
CHAF	Array with current updated fluid pressure heads

CHAI	Previous iteration fluid pressure heads
CON	Species concentrations at the start of the time step
CONF	Species concentrations at the end of the time step
DELT	Time increment
DTMX	Maximum allowable time increment
DTMIN	Minimum allowable time increment
DCAY	First order decay coefficient for species in various phases
DENI	Density of the inert organic component
DIFW	Diffusion coefficient of species in water
DIFO	Diffusion coefficient of species in oil
DIFA	Diffusion coefficient of species in air
DLIQ	Liquid density of pure species
UDENW	Updated density of water phase
DENO	Updated density of oil phase
DENA	Updated density of gas phase
DXX	Dispersion coefficients in the x-direction
DYY	Dispersion coefficients in the y-direction
ECORD(i,1)	x-coordinates of nodes i in the domain
ECORD(i,2)	y-coordinates of nodes i in the domain
EPART	Nonequilibrium partition rate coefficients
ESM	Temporary storage during element stiffness matrix computations
EF	Temporary storage during element stiffness matrix computations

ESN	Temporary storage during element stiffness matrix computations
ESN1	Temporary storage during element stiffness matrix computations
ESMN	Temporary storage during element stiffness matrix computations
ESMN1	Temporary storage during element stiffness matrix computations
ESMNX	Temporary storage during element stiffness matrix computations
GAMA	Equilibrium partition coefficients between phases (see App. A)
HA	Nodal gas pressure at the start of the time step
HAF	Updated gas pressure at nodes
IRUN	Index for execution control (see App. A)
IRES	Restart option index (see App. A)
ICOM	Index describing gas compressibility (see App. A)
ICON	Index for convergence 1 = no convergence and the iteration is repeated;0=solution has converged
ICN	Number of flow BC schedules
IDIM	Index to specify the units of linear dimension (see App. A)
IPROP	Material property to be assigned to the node
IRAD	Index to describe 2-D flow (see App. A)
ITRN	Index to include transport module (see App. A)
IDBC	Array to store number of element and sides subjected to type-3 BC transport module (see App. A)
IFEMC	Index to activate ASD (see App. A)
IMCOR	Index to activate mass injection scheme (see App. A)
IMPE	Serial number of an active element in ASD formulation

JINF	Index for terminating the current run based on cumulative fluid intake
KEQUL	Index to activate kinematic mass transport (see App. A)
KUNIT	Index to specify mass units (see App. A)
KTUDAT	Index to specify updating of mass transfer rates (see App. A)
KCN	Total number of schedules describing transport boundary conditions
KIC	Option for initial condition of transport (see App. A)
KSCH	Schedule for transport boundary conditions
MCNT	Maximum number of iterations allowed
MXTST	Maximum number of time steps allowed
NCM	Node numbers in an element
NPH	Number of phases (see App. A)
NNBi	Nodes and schedules for water (i=1), oil (i=2) and gas (i=3) phases for type-1 flow boundary conditions (see App. A)
NNSp	Elements and side numbers for water (p=W), oil (p=O) and gas (p=A) phases subject to type-2 flow boundary conditions (see App. A)
NTSP	Total number of noninert species
NCON	Total number of type-1 nodes for transport
NEBC	Total number of type-3 elements for transport
NMAT	Total number of material types
NSPB	Number of node with type-1 transport boundary condition
PROP	Material properties (see App. A)
PRON	Temporary storage of element material properties in flow module
PR	Temporary storage of nodal properties in flow module
PHI	Porosity

VXX	x-direction flow velocities at nodes
VYY	y-direction flow velocities at nodes
QFX	Subset of x-direction flow velocities at nodes in an element
QFY	Subset of y-direction flow velocities at nodes in an element
RHOW	Specific gravity of oil phase
RKNA	Relative conductivity of phase at nodes
RHP(1,1)	Density of pure water
RHP(1,2)	Density of inert oil component
RHP(1,3)	Density of uncontaminated air
RW(i,1)	Interphase transfer rate to water phase at node i
RW(i,2)	Interphase transfer rate to oil phase at node i
RW(i,3)	Interphase transfer rate to gas phase at node i
SAW	Updated saturation of water phase
SAO	Updated saturation of oil phase
SAP	Subset of liquid phase saturations
SAWO	Water phase saturation at the start of current time step
SAOO	Oil phase saturation at the start of current time step
SWMN1	Historical minimum saturation at a given location since changing from a two phase air-water to a three phase air-oil-water system
SOT	Saturation of trapped oil
TINF	Cumulative total intake (see App. A)
TIME	Simulation time
TMAX	Maximum simulation time

TMXG	Tolerance for deciding if gas phase is at steady state (see App. A)
TH	Time weighting factor (see App. A)
TFACT	Increment factor for time-step (see App. A)
TOLL	ASD tolerance for liquid pressures (see App. A)
TOL2	ASD tolerance for liquid saturations
TPNT	Time interval for printout of results (see App. A)
TRANS(1)	Longitudinal dispersivity
TRANS(2)	Transverse dispersivity
TTRN	Time at which interphase mass transfer updating starts
URW	Interphase mass transfer rate between oil-water phases
VRA	Interphase mass transfer rate between air-oil/water phases
VRS	Interphase mass transfer rate between water-solid phases
VISAW	Ratio of air to water viscosity
VOL	Area (Cartesian) or volume (radial) of the domain assigned to each node
WFAC	Mass injection rates at nodes
WFNn	Temporary storage for element properties in flow module (n=41, 42)
XCO	x-coordinates of nodes on the x-axis starting from the lower left corner
ZCO	y-coordinates of nodes on the y-axis starting from the lower left corner

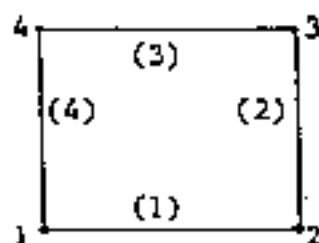


Figure 4.1. Local side numbering of quadrilateral elements.

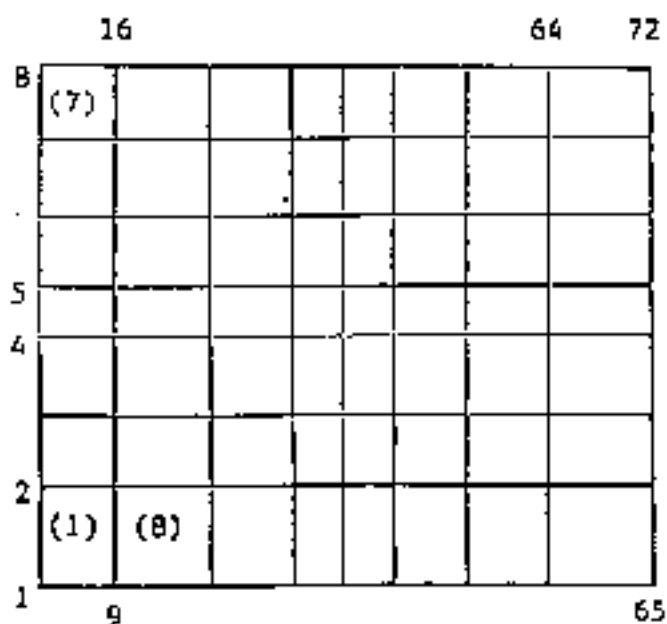


Figure 4.2. Finite element mesh with numbers in parentheses indicating global element numbers and others referring to global node numbers.

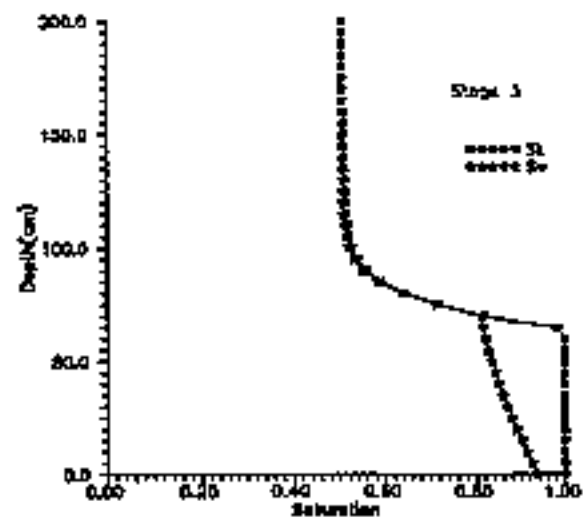
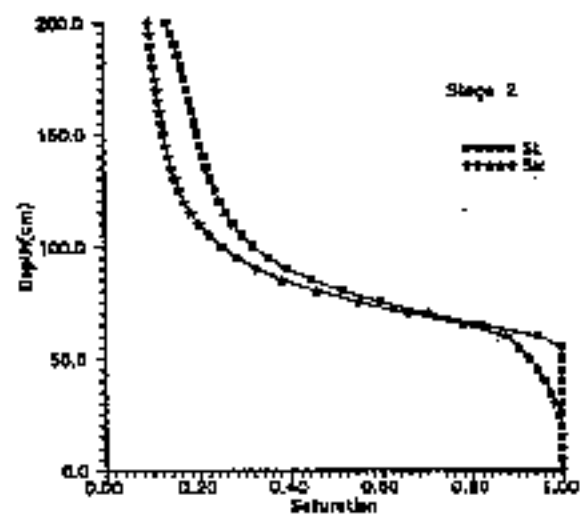
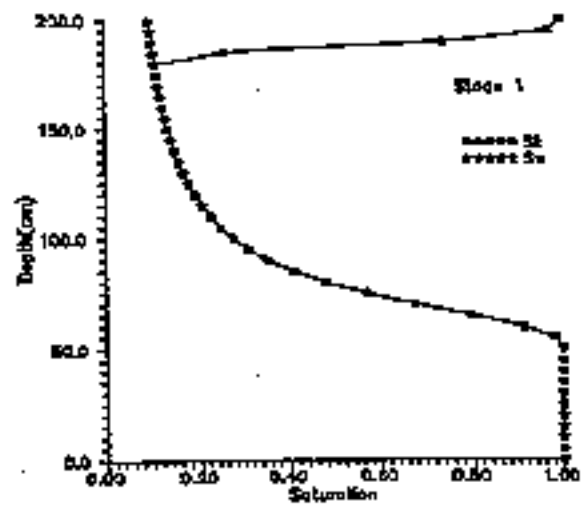


Figure 5.1 Water and total liquid saturation vs depth at end of Stages 1, 2 and 3 for Example 1.

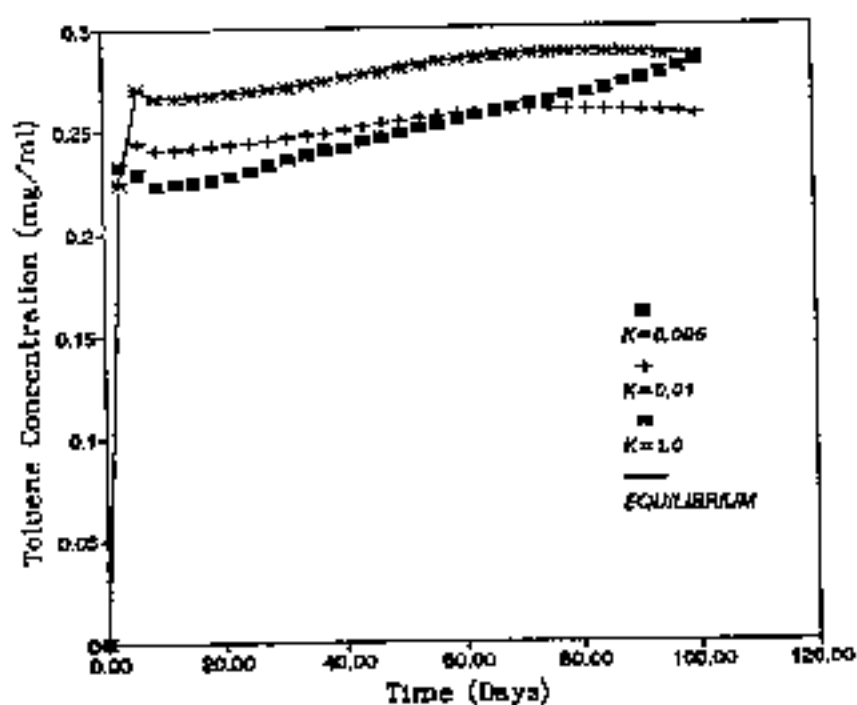
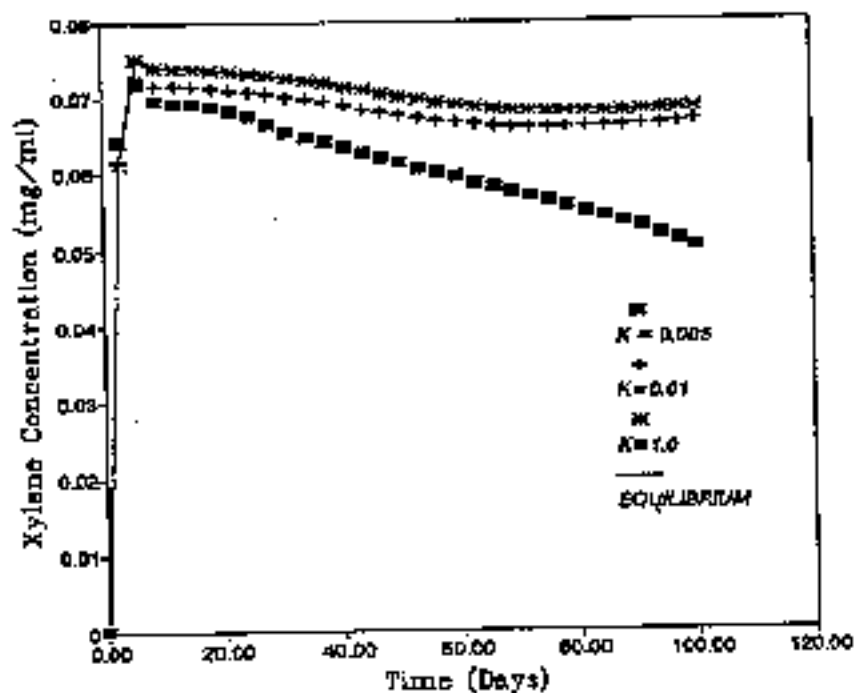


Figure 5.2 Aqueous xylene and toluene concentrations at outflow boundary for Example 1 for equilibrium and nonequilibrium analyses. Rate coefficients in d^{-1} .

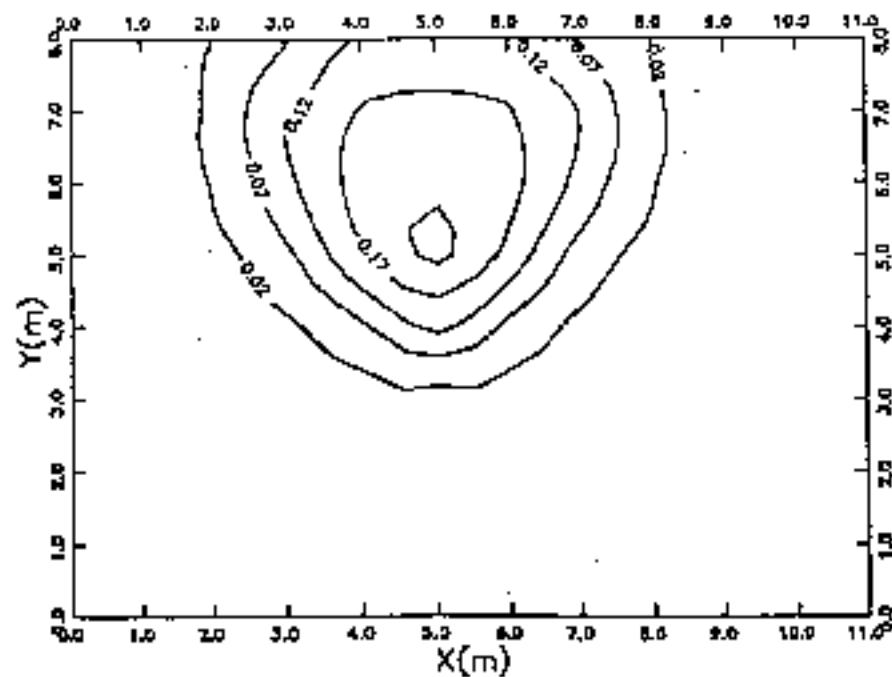


Figure 5.3 Oil saturation contours at the end of Stage 2 for Example 2.

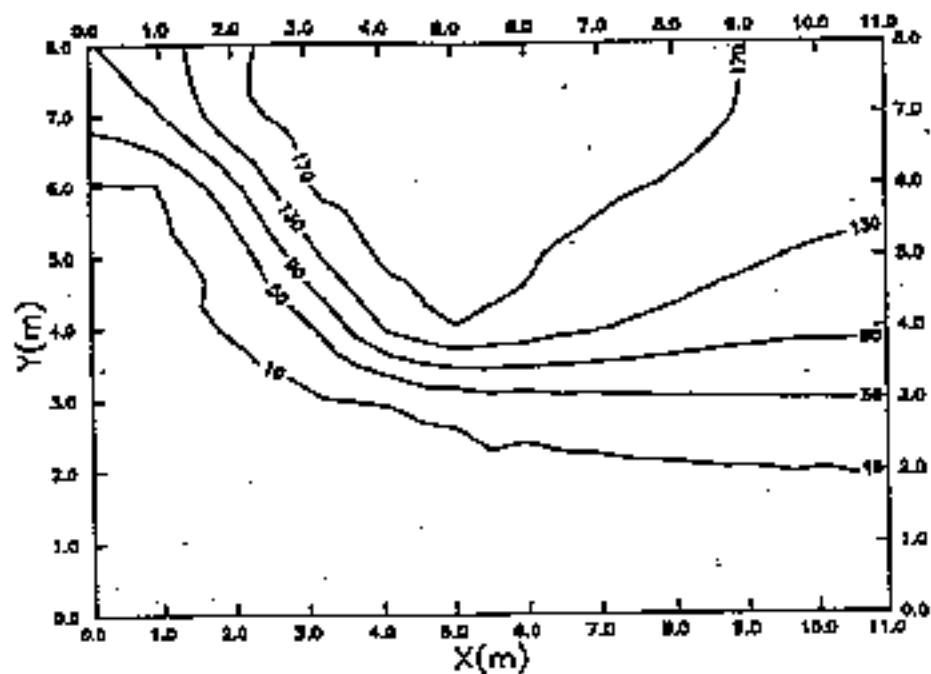


Figure 5.4 Water phase concentration contours (g m^{-3}) at the end of Stage 2 for Example 2.

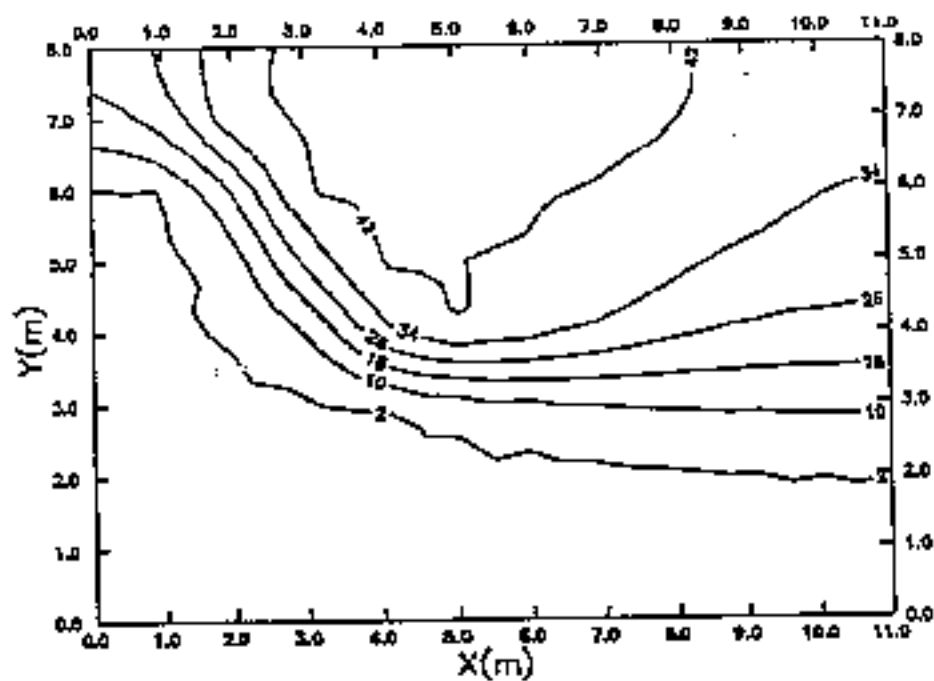


Figure 5.5 Gas phase concentration contours (g m^{-3}) at the end of Stage 2 for Example 2.

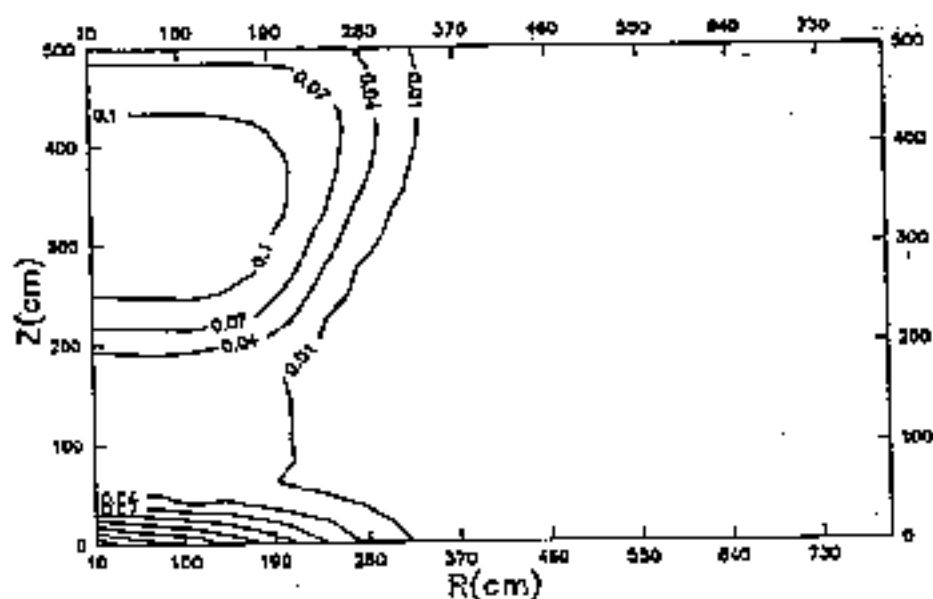


Figure 5.6 Oil saturation contours at the end of Stage 2 for Example 3.

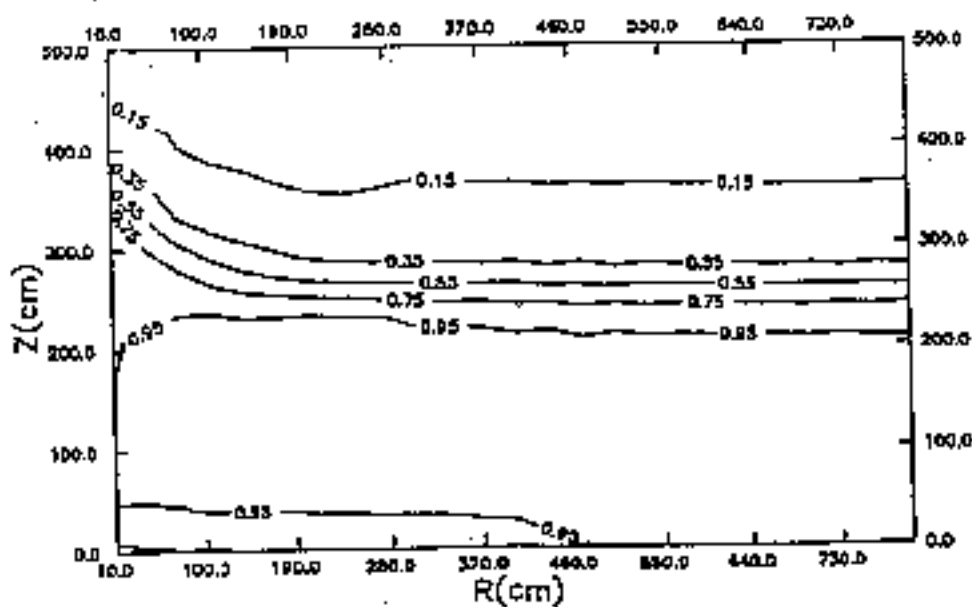


Figure 5.7 Water saturation contours at the end of Stage 3 for Example 3.

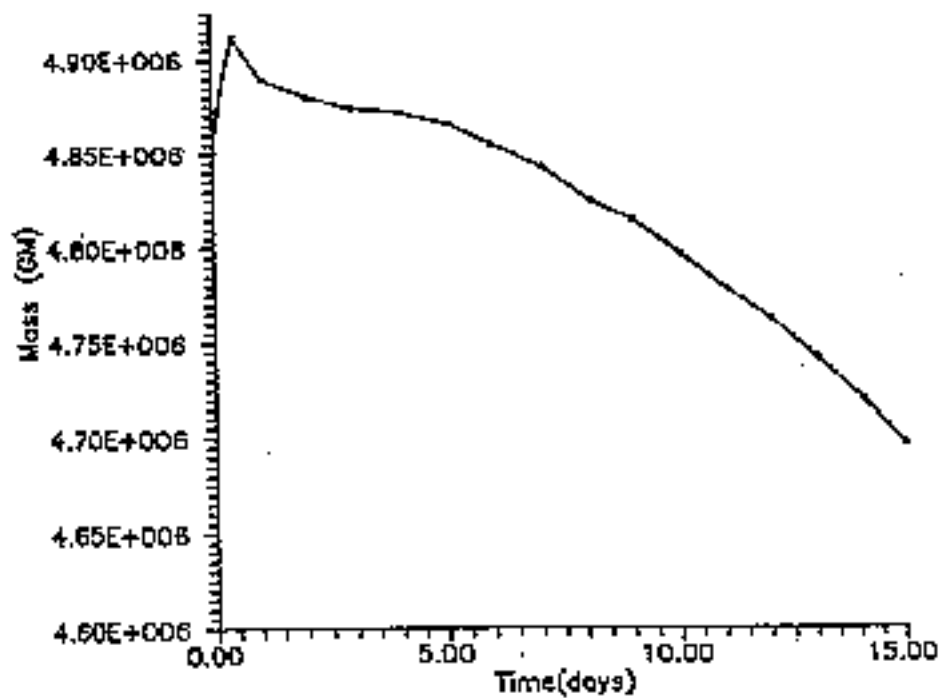


Figure 5.8 PER mass in system vs time during Stage 3 of Example 3.